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Open Notebook Science Challenge Solubilities of Organic Compounds in Organic Solvents

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Open Notebook Science Challenge

Solubilities

of

Organic Compounds

in

Organic Solvents

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and

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Preface

The Open Notebook Science Solubility Challenge

Solubility is an important consideration for many chemistry applications. Synthetic chemists usually use a solvent to perform reactions and knowledge of the solubility of the starting materials or products can be very useful to pick an appropriate solvent. Analytical chemists can use solubility to design separation techniques and factor in dynamic range considerations. Physical chemists can create and evaluate their models of how molecules interact in the solubilization and precipitation processes.

Solubility data can be obtained from a variety of online and offline sources. As with all chemical data, it can be a challenge to evaluate reported measurements. Some databases offer no references while others provide citations to peer reviewed journal articles. Given the choice, more weight is generally given to the latter. This is reasonable in most cases because more information about the purity of compounds and the methods used are available in peer-reviewed articles.

However, the information for how a specific measurement was obtained within a journal article is not generally provided. General methods are provided but the raw data for a specific measurement are typically not published. Peer review is not intended to validate individual measurements - its function is to ensure that the authors made appropriate conclusions based on their processed datasets and the state of knowledge in the field.

The Open Notebook Science Challenge was initiated in the fall of 2008 as the result of a discussion on a train in the UK between Jean-Claude Bradley and Cameron Neylon.[1,2] The concept was very simple: create a crowdsourcing opportunity for the chemistry community to contribute solubility measurements under Open Notebook Science conditions. This method of publication entails providing immediate public access to the chemist's laboratory notebook, as well as all raw data used to compute the measurements.[3,4]

On Sept 3, 2008 the first ONSC measurements were recorded by Bradley and Neylon at the University of Southampton in Neylon's laboratory.[5] The project was soon sponsored by Submeta, offering ten \$500 awards for students in the US or the UK who best recorded how they performed their experiments.[6] Furthermore, the first 3 winners also received one year subscriptions to Nature magazine, thanks to a sponsorship from the Nature Publishing Group.[7] Sigma-Aldrich supported the contest by donating chemicals upon request.[8]

Students were evaluated by a group of judges who convened once a month to deliberate the next award. Judges also provided feedback to the students by commenting on their lab notebook pages directly on the wiki. Their expertise ranged from chemistry to mathematics, spectroscopy and molecular biology.

Techniques

Participants in the ONS Challenge were not required to use a specific method to measure solubility - although they were required to properly document their experiments and analyses. Due to its simplicity, most measurements in the past year were made using the SAMS NMR technique, requiring no volume measurement or calibration curves.[9] Two assumptions are made with this method. The first is that the volume of solute and solvent are additive, with the error becoming negligible at low solubility values. The second is that NMR integration values are proportional to the amount of solvent and solute. Some deviations from this have been observed for default NMR parameters and in later experiments long relaxation times are introduced into the protocol (D1 = 50s).[10]

Data Curation

Since an Open Notebook approach is used in this work, those interested in the validity of the measurements can assess the methods used - both for the preparation of saturated solutions and the raw data from the measurements. Over time, values in the database are likely to improve and possibly some errors may be uncovered and corrected. However, on the whole, we feel that the values provided in this work should be of use to chemists trying to gain an appreciation of solubility for most applications. This is especially the case for values that are not obtainable from any other source.

When clearly erroneous data points are discovered, they are flagged in the database as "DONOTUSE". This way interfaces with the dataset can ignore these values while allowing anyone to investigate why the data points were flagged. This might happen when early experiments did not allow for sufficient mixing or NMR D1 relaxation times were long enough to fully integrate peaks of interest. Out of 681 reported measurements, 51 are currently marked in this way. A shared Google Spreadsheet is used to collect and curate the dataset. This allows easy data entry while providing a simple way to interrogate the database for visualization applications via the Google API.[11]

Literature data and format conversions

An additional 400 solubility measurements from the literature are included in the database. These generally correspond to compounds that are structurally identical or similar to the compounds measured by the ONS Challenge participants. These values are averaged in with the values from the participants, with appropriate references provided. In order to compare values, conversions from molar fraction or g solute/100g solvent to molarity were made by assuming that the volumes are additive and obtaining the density of the solutes in most cases from the predicted values in ChemSpider.[12]

For the convenience of chemists with diverse applications, all three formats are provided. For the cases where solutes are miscible with the solvent, the molarity reported is simply the solute's density. The practical interpretation of this is that solutions of any molarity below the solute's density can be prepared.

In the process of converting units and averaging heterogeneous data sources, no attempt has been made to track significant figures.

Those interested in any information about the precision of measurements should consult each individual data source. This may not be an easy task for measurements only carried out once and where factors such as the quality of spectral peaks and baselines are not optimal.

This collection will be most valuable for those who do not require highly precise measurements for their applications. For example, synthetic chemists can easily use rough estimates of solubility to select appropriate solvents for a reaction. In any case, one would be wise to consider all measurements as provisional, regardless of the source. As more data are collected, subsequent editions of this book will adjust values accordingly.

Predicted Solubilities

Predicted solubility values for selected solutes in a range of solvents are provided in a section. Specifically, solutes are included when measurements from at least 5 different solvents are available. A method using Abraham descriptors depends on the experimental solubility measurements from several solvents to make predictions, which is detailed in that section of the book. For this reason, some aqueous solubility measurements are included, which are generally available from the literature. Predicted aqueous solubilities are used when experimental values are not available. The focus of this collection remains on non-aqueous solubility.

Consistent with how the experimental measurements are made available, the predicted solubility values are provided as a work in progress. The purpose in providing them is to suggest solvents of interest for various applications. The boiling point of each solvent is also listed in the table to allow a convenient selection. When available, experimental measurements are listed next to the predicted values. This information can be helpful to gauge the usefulness of the model to some extent but does not guarantee its reliability for the other solvents. As more measurements are collected the reliability of the predictions is likely to increase and this will be reflected in future editions of this book.

Searching the database

The values in this database can be accessed and filtered in various ways. More information is available at the ONS Challenge wiki[13] and Chapter 16 of the book "Beautiful Data".[14]

Database version

Archived as an Excel Spreadsheet by WebCite on February 11, 2010.[15]

Notebook archive

This is the first edition to include a full archive of the ONS Challenge notebook. A space export from Wikispaces provides an initial version of all the HTML pages in the notebook with local hyperlinks to copies of all images and files uploaded onto the wiki. All of the Google Spreadsheets are automatically downloaded as Excel spreadsheets and placed in the same "files" folder as the images. NMR spectra, stored as JCAMP-DX files, are placed in the "spectra" folder. All of the HTML pages are reformatted to provide local references to both Excel spreadsheets and the JCAMP-DX files.

The notebook archive is meant to represent a snapshot of the state of all source documents at the time of the publication of an edition of this book. When used from a server with web services running, clicking on links to the spectra will allow interaction via a browser interface, including zooming in or out and integration of the NMR spectrum. When accessed in stand-alone mode after downloading or directly from a CD, everything will work the same, except that JCAMP-DX files must be open from JSpecView running on the desktop. Excel files will retain any calculations in the cells of the original Google Spreadsheets but dynamic values generated from calling web services - such the script that automatically integrates NMR spectra - will be frozen as simple values. However the link to the web service used will be stored in the cell as a comment. Links to external websites are not crawled and embedded Google Spreadsheets or videos are not copied. These will work but will reflect live data on the web.

The February 11, 2010 version of the notebook archive is available on a hosted site[16], on a CD[17] or by download[18].

References

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Judges



Jean-Claude Bradley is an Associate Professor of Chemistry and E-Learning Coordinator for the College of Arts and Sciences at Drexel University. He leads the UsefulChem project, an initiative started in the summer of 2005 to make the scientific process as transparent as possible by publishing all research work in real time to a collection of public blogs, wikis and other web pages. Jean-Claude coined the term Open Notebook Science to distinguish this approach from other more restricted forms of Open Science. Jean-Claude teaches undergraduate organic chemistry courses with most content freely available on public blogs, wikis, games, Second Life and audio and video podcasts. He has a Ph.D. in organic chemistry and has published articles and obtained patents in the areas of synthetic and mechanistic chemistry, gene therapy, nanotechnology and scientific knowledge management. <http://usefulchem.blogspot.com>



Cameron Neylon is a biophysicist who has always worked in interdisciplinary areas and is an advocate of open research practice and improved data management. He currently works as Senior Scientist in Biomolecular Sciences at the ISIS Neutron Scattering facility at the Science and Technology Facilities Council (STFC). Along with his work in structural biology and biophysics his research and writing focuses on the interface of web technology with science and the successful (and unsuccessful) application of generic and specially designed tools in the academic research environment. He is a founder member of the Open Knowledge Foundation Science Working Group and writes regularly on Open Research at his blog, Science in the Open. <http://blog.openwetware.org/scienceintheopen>



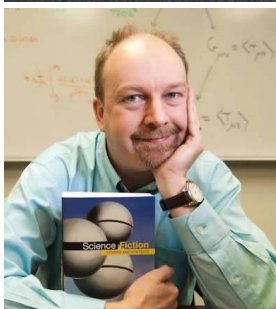
Rajarshi Guha is a Research Scientist at the NIH Chemical Genomics Center (NCGC). At the NCGC he is involved in cheminformatics methodology and software development for various aspects of high throughput screening for small molecules and RNAi. His research makes extensive use of statistical methods and has been applied to a variety of biological systems. Along with algorithm development, he is extensively involved in cheminformatics software development, including development of toolkits, web services and integration of these into distributed infrastructures. As a believer in Open Source and Open Data, much of his research and software is available under Open Source licenses. <http://blog.rguha.net>



Antony Williams is the host of ChemSpider, the online chemistry portal leading the charge towards open and collaborative chemistry. ChemSpider provides access to over 23 million unique chemical entities sourced from almost 300 data sources and provides a platform for community based depositions and curation to clean up internet-based chemistry. Antony spent over a decade in the commercial scientific software business as Chief Science Officer for a Cheminformatics software company and during his tenure oversaw their product development, marketing and sales teams. He is an accomplished NMR spectroscopist with over 100 peer-reviewed publications. During his career he was the NMR Technology Leader for the Eastman-Kodak company and has worked in both academia and national government research institutions. He has recently taken his passion for providing access to chemistry related information and software services to the masses by hosting the ChemSpider service. <http://www.chemspider.com/blog/>



Bill Hooker is a molecular biologist by trade and has worked on G protein signaling, PCR diagnostics, anti-schistosome vaccines, HIV replication and molecular mechanisms of cancer. He serves as an associate editor on the innovative Open Access journal BioMed Central Research Notes and as a member of the advisory board of the Berglund Center for Internet Studies. He is currently the R&D team leader at a small biotech company in Portland, OR. He has never had an idea that couldn't be improved by sharing it with as many people as possible, and doesn't believe that anyone else has, either. He is particularly interested in extending the "open" ethos of Open Source software and Open Access publishing to all aspects of science, from raw data to hypothesis testing by way of distributed, collaborative effort. <http://www.sennoma.net>



Andrew Lang is a Professor of Mathematics at Oral Roberts University. His PhD training is in the area of quantum field theory in curved spacetime. While remaining active in this area he has always enjoyed working collaboratively on interdisciplinary projects ranging from modeling basketball free throws to the stability of spinning spacecraft under thrust. His interests include the relationship between science and science fiction and the epistemological differences between teleology and metaphysical naturalism. As a result of being a judge for the Open Notebook Science Challenge he has developed an appreciation for openness in science, multi-dimensional data visualization and cheminformatics. http://webapps.oru.edu/new_php/blog/index.php?user_id=23

Educational Partners



J. Brent Friesen from Dominican University incorporated the Open Notebook Science Solubility Challenge into his Sophomore Organic Chemistry laboratory course in January 2009. He has been a professor in the natural science department at Dominican University since 1999. He regularly teaches Organic Chemistry (lecture and laboratory), Biochemistry, Introduction to Organic Chemistry, Chemistry of Natural Products, and Forensic Chemistry. His research focuses on the automation of countercurrent separation technology, anti-tuberculosis compounds, and interactions with Reichardt's Dye. Friesen has also done research with undergraduates on projects such as "Biorenewable Solvents for Countercurrent Chromatography" and "Used Coffee Grounds: A New Source of Biofuels." Friesen is a regular volunteer with the Oak Park Education Foundation's Global Village, a program matching scientists with elementary school classrooms. His recent articles include "Saying What You Mean: Teaching Mechanisms in Organic Chemistry" (Journal of Chemical Education) and "Countercurrent Separation of Natural Products" (Journal of Natural Products).

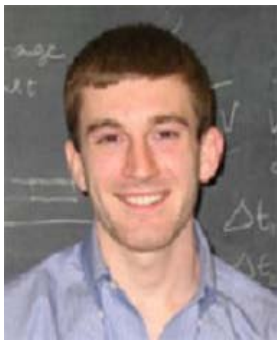
Students



Tim Bohinski (April 2009 Submeta Award winner) is a senior at Drexel University majoring in chemistry, with a strong interest in organic and theoretical chemistry. He will be graduating with a B.S. in June 2010. He is currently performing undergraduate research in the theoretical/physical field, studying nanoparticle optics, specifically in the area of plasmoms. He plans to continue his studies at the doctorate level. Tim is also a member of the Drexel American Chemical Society and was a member of the Drexel Crew Team. In my spare time he enjoys the outdoors, staying fit, and homebrewing. LinkedIn profile: <http://www.linkedin.com/pub/timothy-bohinski/18/110/a7> Supervisor: Jean-Claude Bradley, Drexel



David Bulger (February 2009 Submeta Award winner) is a junior Chemistry major at Oral Roberts University in Tulsa, OK. Since freshman year, he has been involved in research ranging from water purity, red tide in Second Life, collaboration between water utilities and academia, NMR solubility determination and Sortase A inhibition. After his undergraduate degree, he plans to pursue an M.D. or M.D./Ph.D. http://biolab.isis.rl.ac.uk/david_bulger. Supervisor: Robert Stewart, Oral Roberts University



Matthew Federici (June 2009 Submeta Award winner) graduated from the University of Virginia in 2008. After receiving the Naval ROTC Tweeddale Scholarship Award in 2004, Matthew studied naval nuclear engineering and interned on the USS Alexandria. As a varsity student athlete, he doubled majored in mechanical engineering as well as aerospace engineering. Matthew spent his senior year at UVA studying biomechanics under Dr. Pradip Sheth. His undergraduate academic career finished by winning the Cyrus Society Award, given to a select few of student athletes with outstanding academic performance and community service. Matthew is pursuing his PhD in Mechanical Engineering under Dr. Minjun Kim at Drexel University. As a GAANN fellow, he is currently investigating biomimetics and drug delivery systems. Matthew plans to attend medical school following the completion of his dissertation. Website: <http://microfluidics.tripod.com/> **Supervisor: Jean-Claude Bradley, Drexel**



Jennifer (Jenny) Hale (December 2008 Submeta Award winner) gained a BSc in Chemistry with Pharmacology from the University of Southampton, UK, in 2004. Following her degree she spent 15 months working on the synthesis of phosphoramidites before taking up a PhD in the department of chemical biology in 2006. Jenny's area of research for her PhD has been the directed evolution of a beta-glucuronidase into a beta-galactosidase via neutral drift, a phenomenon found in natural evolution that has only recently begun to be explored in laboratory evolution. Additionally, her research has been used in the development and testing of an electronic laboratory notebook in the form of a blog: LaBLog (http://blogs.chem.soton.ac.uk/neutral_drift) as well as wider investigations into Open Notebook Science. Outside of the laboratory, Jenny is a keen ballroom and latin dancer and spent a year as president of the Southampton University Ballroom and Latin Dance Society, as well as competing in numerous university dancesport competitions. **Supervisor: Cameron Neylon, Southampton**



Jenna Mancinelli (September 2009 Submeta Award winner) is currently a junior at Drexel University, studying Biology. She is particularly interested in human physiology and its relation to clinical medicine. She hopes to attend medical school following her graduation from Drexel University. In her spare time, Jenna enjoys going to concerts, studying Italian and experimenting with her culinary skills. **Supervisor: Jean-Claude Bradley, Drexel**



Khalid Baig Mirza (January 2009 Submeta Award winner) obtained a BSc in Chemistry and Biology from Osmania University, India. He earned an MS in Chemistry from Fairleigh Dickinson University at Madison, NJ in 2002. He is currently working towards a PhD at Drexel University under the guidance of Prof. Jean-Claude Bradley. His research focuses on the synthesis of potentially active anti-malarial diamides obtained from a Ugi reaction. His research is performed in the open as 'Open Notebook Science'. He enjoys gardening, cricket and keeping up to date on world affairs. **Supervisor: Jean-Claude Bradley, Drexel**



Marshall Moritz (July 2009 Submeta Award winner) is a chemistry and mathematics double major at Syracuse University in Syracuse, NY with an anticipated graduation in May 2011. After studying abroad in Hong Kong, he is looking forward to continuing his studies at SU and pursuing further research not only in solubility determination by NMR but also in other areas of organic chemistry. Following graduation, he hopes to continue his education in graduate school with a masters degree. He is an avid cyclist, cycling cross country in 2006, and is also a traveling and music enthusiast. **Supervisor: Jean-Claude Bradley, Drexel**



Daniel Rein (August 2009 Submeta Award winner) is currently a student studying chemistry and biology at Drexel University. He plays guitar in Jazz Band and is passionate about music. For freshman year he studied physics at Northeastern. <http://www.linkedin.com/pub/daniel-rein/18/31a/72b> **Supervisor: Jean-Claude Bradley, Drexel**



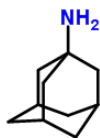
Cedric Tchakounte (March 2009 Submeta Award winner) is a senior majoring in Biological Sciences & Biotechnology at Drexel University. He is a distinguished student, having received multiple Dean's List honors and the Who's Who Among Students in American Universities & Colleges award. He has also shown his dedication to community and service by being a mentor for Guided Youths. He enjoys performing research, because he believes it to be a cornerstone to learning true science. With his academic chapter as an undergraduate coming to an end, Cedric looks forward to what awaits. He plans on pursuing a career in medicine. **Supervisor: Jean-Claude Bradley, Drexel**



Hai Truong (December 2009 Submeta Award winner) is pursuing a BS in Chemistry at Drexel University from 2009. After graduating with honors from a high school for the Gifted in Vietnam, he came to the United States for college. In 2008, he attended Collin College in McKinney, TX. At Collin, he was a member of Phi Theta Kappa, an international honor society for two-year colleges. In 2009, he transferred to Drexel University with a Dean's Scholarship. Beside academic studies, Hai enjoys swimming and playing tennis. **Supervisor: Jean-Claude Bradley, Drexel**

Solubilities

1-adamantylamine $C_{10}H_{17}N$



Compound Data

Molecular weight	151.249	H bond acceptors	1	Rule of 5 violations	0
Compound type	amine	H bond donors	2	ACD/ALogP	2.22
Phase 25°C	solid	Rotatable bonds	1	Predicted density	1.066 g/cm ³
SMILES	<chem>C1C2CC3CC1CC(C2)(C3)N</chem>				
InChIKey	DKNWSYNQZKUICI-UHFFFAOYSA-N				

Solubility Data

Solvent	Concentration (M)	Mole Fraction (X)	pph (g/100g)
methanol	0.36	0.02	7.62

1-octadecylamine $C_{18}H_{39}N$ ^{69, 908}

Compound Data

Molecular weight	269.509	H bond acceptors	1	Rule of 5 violations	1
Compound type	amine	H bond donors	2	ACD/ALogP	8.37
Phase 25°C	solid	Rotatable bonds	17	Predicted density	0.818 g/cm ³
SMILES	<chem>CCCCCCCCCCCCCCCCCC</chem>				

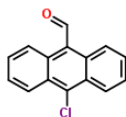


InChIKey REYJPSVUYRZGE-UHFFFAOYSA-N

Solubility Data

Solvent	Concentration (M)	Mole Fraction (X)	pph (g/100g)
acetonitrile	0.08	0.00	2.96
ethanol	1.77	0.20	146.72
hexane	0.13	0.02	5.42
methanol	1.68	0.14	134.67
THF	1.68	0.23	112.18
toluene	1.34	0.20	74.24

10-chloro-9-anthraldehyde C₁₅H₉ClO⁵⁷

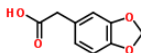


Compound Data			
Molecular weight	240.684	H bond acceptors	1
Compound type	aldehyde	H bond donors	0
Phase 25°C	solid	Rotatable bonds	1
SMILES	O=Cc2c1c(cccc1)c(Cl)c3c2ccccc3		
InChIKey	SHYBXXMECBHHFH-UHFFFAOYSA-N		

Solubility Data

Solvent	Concentration (M)	Mole Fraction (X)	pph (g/100g)
ethanol	0.00	0.00	0.00
methanol	0.00	0.00	0.00
THF	0.08	0.01	2.16

2-(1,3-benzodioxol-5-yl)acetic acid C₉H₈O₄^{98, 82}



Compound Data			
Molecular weight	180.157	H bond acceptors	4
Compound type	carboxylic acid	H bond donors	1
Phase 25°C	solid	Rotatable bonds	2
SMILES	O=C(O)Cc1ccc2OCOc2c1		
InChIKey	ODVLMCWNGKLROU-UHFFFAOYSA-N		

Solubility Data

Solvent	Concentration (M)	Mole Fraction (X)	pph (g/100g)
acetonitrile	0.67	0.04	17.68
DMSO	5.37	0.55	282.22
THF	2.73	0.25	83.68

2-(4-hydroxyphenyl-azo)benzoic acid C₁₃H₁₀N₂O₃^{3, 32}



Compound Data			
Molecular weight	242.23	H bond acceptors	5
Compound type	carboxylic acid	H bond donors	2
Phase 25°C	solid	Rotatable bonds	4
SMILES	Oc2ccc(N=Nc1ccccc1C(=O)O)cc2		
InChIKey	DWQOTEPNRWVUDA-CCEZHUSRSA-N		

Solubility Data

Solvent	Concentration (M)	Mole Fraction (X)	pph (g/100g)
ethanol	0.09	0.01	2.68
methanol	0.06	0.00	1.95
THF	0.55	0.05	16.42

2-chloro-5-nitrobenzaldehyde C₇H₄ClNO₃^{105, 69, 208, 33, 205}



Compound Data

Molecular weight	185.565	H bond acceptors	4	Rule of 5 violations	0
Compound type	aldehyde	H bond donors	0	ACD/ALogP	2.5
Phase 25°C	solid	Rotatable bonds	2	Predicted density	1.485 g/cm ³
SMILES	<chem>O=Cc1cc(ccc1Cl)[N+](=O)[O-]</chem>				
InChIKey	VFVHWCKUHAEDMY-UHFFFAOYSA-N				

Solubility Data

Solvent	Concentration (M)	Mole Fraction (X)	pph (g/100g)
acetonitrile	2.31	0.15	80.47
chloroform	2.90	0.27	56.27
DMSO	2.93	0.25	78.05
ethanol	*	*	*
methanol	*	*	*
THF	2.79	0.25	87.80
toluene	1.74	0.19	47.44

* This aldehyde reacts with alcohols to form a hemiacetal.

2-chloro-5-nitrobenzoic acid C₇H₄ClNO₄⁹⁰⁵



Compound Data

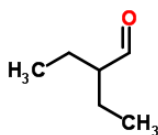
Molecular weight	201.564	H bond acceptors	5	Rule of 5 violations	0
Compound type	carboxylic acid	H bond donors	1	ACD/ALogP	2.02
Phase 25°C	solid	Rotatable bonds	2	Predicted density	1.602 g/cm ³
SMILES	<chem>O=C(O)c1cc(ccc1Cl)[N+](=O)[O-]</chem>				
InChIKey	QUEKGYQTRJVEQC-UHFFFAOYSA-N				

Solubility Data

Solvent	Concentration (M)	Mole Fraction (X)	pph (g/100g)
1-butanol	0.78	0.07	21.66
1-decanol	0.39	0.07	9.98
1-heptanol	0.54	0.08	14.24
1-hexanol	0.64	0.08	17.19
1-octanol	0.48	0.07	12.51
1-pentanol	0.74	0.08	20.28
1-propanol	0.95	0.08	27.36
2-butanol	0.91	0.09	25.86
2-methyl-1-propanol	0.63	0.06	17.22
2-methyl-2-propanol	1.21	0.12	35.78
2-pentanol	0.76	0.08	20.94
2-propanol	1.13	0.09	33.57
3-methyl-1-butanol	0.68	0.07	18.53
butyl acetate	0.46	0.06	11.11
dibutyl ether	0.10	0.02	2.62
diethyl ether	0.57	0.06	16.86
diisopropyl ether	0.19	0.03	5.18
ethanol	1.40	0.09	43.91
ethyl acetate	0.75	0.08	18.59
methyl acetate	0.89	0.08	22.25

pentyl acetate	0.43	0.06	10.39
THF	2.97	0.27	105.73

2-ethylbutyraldehyde C₆H₁₂O²²



Compound Data

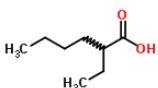
Molecular weight	100.159	H bond acceptors	1	Rule of 5 violations	0
Compound type	aldehyde	H bond donors	0	ACD/ALogP	1.79
Phase 25°C	liquid	Rotatable bonds	3	Predicted density	0.799 g/cm ³
SMILES	O=CC(CC)CC				
InChIKey	UNNGUFMVYQJGTD-UHFFFAOYSA-N				

Solubility Data

Solvent	Concentration (M)	Mole Fraction (X)	pph (g/100g)
methanol	8.13	□	□

□ Solute is very soluble/miscible, conversion fail.

2-ethylhexanoic acid C₈H₁₆O₂²²



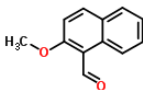
Compound Data

Molecular weight	144.211	H bond acceptors	2	Rule of 5 violations	0
Compound type	carboxylic acid	H bond donors	1	ACD/ALogP	2.72
Phase 25°C	liquid	Rotatable bonds	5	Predicted density	0.926 g/cm ³
SMILES	O=C(O)C(CC)CCCC				
InChIKey	OBETXYAYXDNJHR-UHFFFAOYSA-N				

Solubility Data

Solvent	Concentration (M)	Mole Fraction (X)	pph (g/100g)
methanol	6.26	0.91	4777.15

2-methoxy-1-naphthaldehyde C₁₂H₁₀O₂²⁰⁵



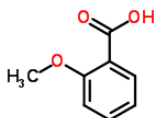
Compound Data

Molecular weight	186.207	H bond acceptors	2	Rule of 5 violations	0
Compound type	aldehyde	H bond donors	0	ACD/ALogP	2.95
Phase 25°C	solid	Rotatable bonds	2	Predicted density	1.169 g/cm ³
SMILES	O=Cc1c2c(ccc1OC)ccccc2				
InChIKey	YIQLTKAOHRZOL-UHFFFAOYSA-N				

Solubility Data

Solvent	Concentration (M)	Mole Fraction (X)	pph (g/100g)
methanol	1.26	0.06	38.98

2-methoxybenzoic acid C₈H₈O₃^{905, 34, 907}



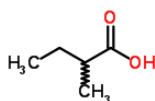
Compound Data

Molecular weight	152.147	H bond acceptors	3	Rule of 5 violations	0
Compound type	carboxylic acid	H bond donors	1	ACD/ALogP	1.5
Phase 25°C	solid	Rotatable bonds	2	Predicted density	1.207 g/cm ³
SMILES	O=C(O)c1ccccc1OC				
InChIKey	ILUJQPXNXACGAN-UHFFFAOYSA-N				

Solubility Data

Solvent	Concentration (M)	Mole Fraction (X)	pph (g/100g)
1-butanol	0.57	0.05	11.61
1-decanol	0.22	0.04	4.16
1-heptanol	0.34	0.05	6.59
1-hexanol	0.37	0.05	7.24
1-octanol	0.30	0.05	5.76
1-pentanol	0.47	0.05	9.37
1-propanol	0.76	0.06	16.09
1,4-dioxane	1.53	0.14	28.99
2-butanol	0.50	0.05	10.14
2-ethyl-1-hexanol	0.25	0.04	4.78
2-methyl-1-butanol	0.39	0.04	7.71
2-methyl-1-pentanol	0.35	0.04	6.84
2-methyl-1-propanol	0.41	0.04	8.21
2-methyl-2-propanol	0.53	0.05	10.75
2-pentanol	0.39	0.04	7.71
2-propanol	0.59	0.05	12.26
3-methyl-1-butanol	0.36	0.04	7.09
4-methyl-2-pentanol	0.32	0.04	6.26
butyl acetate	0.34	0.04	6.10
chloroform	0.46	0.04	5.01
dibutyl ether	0.04	0.01	0.78
diethyl ether	0.24	0.02	5.13
diisopropyl ether	0.06	0.01	1.21
ethanol	1.19	0.08	27.31
ethyl acetate	5.63	0.66	328.57
methanol	1.82	0.09	47.72
methyl acetate	0.86	0.07	16.16
pentyl acetate	0.26	0.04	4.64
propylene carbonate	0.99	0.13	14.28
THF	2.02	0.18	45.61
water	0.03	0.00	0.46

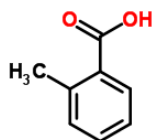
2-methyl butyric acid C₅H₁₀O₂²²



Compound Data				
Molecular weight	102.132	H bond acceptors	2	Rule of 5 violations 0
Compound type	carboxylic acid	H bond donors	1	ACD/ALogP 1.13
Phase 25°C	liquid	Rotatable bonds	2	Predicted density 0.962 g/cm ³
SMILES	O=C(O)C(C)CC			
InChIKey	WLAMNBDJUVNPJU-UHFFFAOYSA-N			

Solubility Data			
Solvent	Concentration (M)	Mole Fraction (X)	pph (g/100g)
methanol	9.16	0.93	4515.12

2-methylbenzoic acid C₈H₈O₂^{905, 907}

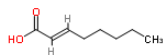


Compound Data				
Molecular weight	136.148	H bond acceptors	2	Rule of 5 violations 0
Compound type	carboxylic acid	H bond donors	1	ACD/ALogP 2.36
Phase 25°C	solid	Rotatable bonds	1	Predicted density 1.151 g/cm ³
SMILES	O=C(O)c1ccccc1C			
InChIKey	ZWLPBLYKEWSWPD-UHFFFAOYSA-N			

Solubility Data			
Solvent	Concentration (M)	Mole Fraction (X)	pph (g/100g)

1-butanol	1.61	0.15	33.64
1-decanol	1.04	0.18	19.50
1-heptanol	1.28	0.18	25.04
1-hexanol	1.38	0.17	27.52
1-octanol	1.16	0.18	22.24
1-pentanol	1.49	0.16	30.37
1-propanol	1.77	0.14	38.34
1,4-dioxane	2.64	0.25	52.53
2-butanol	1.75	0.17	37.51
2-methyl-1-butanol	1.25	0.14	24.69
2-methyl-1-propanol	1.28	0.12	25.64
2-methyl-2-propanol	2.19	0.21	50.05
2-pentanol	1.68	0.19	35.28
2-propanol	1.95	0.16	43.63
3-methyl-1-butanol	1.34	0.15	26.80
4-methyl-2-pentanol	1.39	0.17	27.93
butyl acetate	1.17	0.15	20.87
dibutyl ether	0.58	0.09	10.87
diethyl ether	1.65	0.17	38.03
diisopropyl ether	0.86	0.11	17.20
ethanol	2.08	0.14	48.15
ethyl acetate	1.49	0.15	27.42
methyl acetate	1.51	0.13	27.56
pentyl acetate	1.04	0.15	18.31
propylene carbonate	0.46	0.06	5.50
THF	2.92	0.26	67.18
water	0.01	0.00	0.14

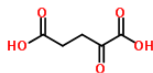
2-octenoic acid C₈H₁₄O₂²²



Compound Data			
Molecular weight	142.196	H bond acceptors	2 Rule of 5 violations 0
Compound type	carboxylic acid	H bond donors	1 ACD/ALogP 2.93
Phase 25°C	liquid	Rotatable bonds	5 Predicted density 0.955 g/cm ³
SMILES	O=C(O)/C=C/CCCC		
InChIKey	CWMPPVPFLSZGCY-VOTSOKGWSA-N		

Solubility Data			
Solvent	Concentration (M)	Mole Fraction (X)	pph (g/100g)
methanol	6.64	0.96	11068.64

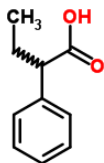
2-oxopentanedioic acid C₅H₆O₅²⁵



Compound Data			
Molecular weight	146.098	H bond acceptors	5 Rule of 5 violations 0
Compound type	carboxylic acid	H bond donors	2 ACD/ALogP -1.43
Phase 25°C	solid	Rotatable bonds	4 Predicted density 1.499 g/cm ³
SMILES	O=C(O)C(=O)CCC(=O)O		
InChIKey	KPGXRSRHYNQIFN-UHFFFAOYSA-N		

Solubility Data			
Solvent	Concentration (M)	Mole Fraction (X)	pph (g/100g)
ethanol	2.99	0.20	79.04
methanol	5.02	0.29	190.70
THF	3.12	0.26	72.46

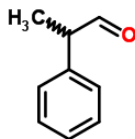
2-phenylbutyric acid C₁₀H₁₂O₂^{79, 83}



Compound Data			
Molecular weight	164.201	H bond acceptors	2 Rule of 5 violations 0
Compound type	carboxylic acid	H bond donors	1 ACD/ALogP 2.38
Phase 25°C	solid	Rotatable bonds	3 Predicted density 1.09 g/cm ³
SMILES	O=C(O)C(c1ccccc1)CC		
InChIKey	OFJWFSNDPCAWDK-UHFFFAOYSA-N		

Solubility Data			
Solvent	Concentration (M)	Mole Fraction (X)	pph (g/100g)
acetonitrile	6.18	0.83	1968.04
DMSO	5.97	0.81	886.12
ethanol	6.20	0.85	1977.18
THF	5.96	0.82	1059.60
toluene	5.35	0.74	519.73

2-phenylpropanal C₉H₁₀O²¹

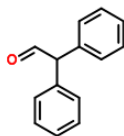


Compound Data			
Molecular weight	134.175	H bond acceptors	1 Rule of 5 violations 0
Compound type	aldehyde	H bond donors	0 ACD/ALogP 2.13
Phase 25°C	liquid	Rotatable bonds	2 Predicted density 0.98 g/cm ³
SMILES	c1ccccc1C(C)C=O		
InChIKey	IQVAERDLDAZARL-UHFFFAOYSA-N		

Solubility Data			
Solvent	Concentration (M)	Mole Fraction (X)	pph (g/100g)
methanol	7.53	□	□

□ Solute is very soluble/miscible, conversion fail.

2,2-diphenylacetaldehyde C₁₄H₁₂O²¹

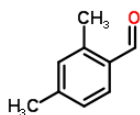


Compound Data			
Molecular weight	196.245	H bond acceptors	1 Rule of 5 violations 0
Compound type	aldehyde	H bond donors	0 ACD/ALogP 3.67
Phase 25°C	liquid	Rotatable bonds	3 Predicted density 1.069 g/cm ³
SMILES	c1ccccc1C(c1ccccc1)C(=O)		
InChIKey	HLLGFGBLKOIZOM-UHFFFAOYSA-N		

Solubility Data			
Solvent	Concentration (M)	Mole Fraction (X)	pph (g/100g)
methanol	5.64	□	□

□ Solute is very soluble/miscible, conversion fail.

2,4-dimethylbenzaldehyde C₉H₁₀O²¹

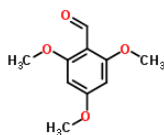


Compound Data			
Molecular weight	134.175	H bond acceptors	1 Rule of 5 violations 0
Compound type	aldehyde	H bond donors	0 ACD/ALogP 2.56
Phase 25°C	liquid	Rotatable bonds	1 Predicted density 1.003 g/cm ³
SMILES	O=Cc1ccc(C)cc1C		
InChIKey	GISVICWQYMUPJF-UHFFFAOYSA-N		

Solubility Data			
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Solvent	Concentration (M)	Mole Fraction (X)	pph (g/100g)
methanol	7.17	0.88	3128.10

2,4,6-trimethoxybenzaldehyde C₁₀H₁₂O₄⁸²



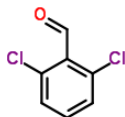
Compound Data

Molecular weight	196.2	H bond acceptors	4	Rule of 5 violations	0
Compound type	aldehyde	H bond donors	0	ACD/ALogP	1.49
Phase 25°C	solid	Rotatable bonds	4	Predicted density	1.133 g/cm ³
SMILES	<chem>O=Cc1c(OC)cc(OC)cc1OC</chem>				
InChIKey	CRBZVDLXAIFERF-UHFFFAOYSA-N				

Solubility Data

Solvent	Concentration (M)	Mole Fraction (X)	pph (g/100g)
THF	0.14	0.01	3.11

2,6-dichlorobenzaldehyde C₇H₄Cl₂O^{208, 205}



Compound Data

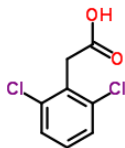
Molecular weight	175.012	H bond acceptors	1	Rule of 5 violations	0
Compound type	aldehyde	H bond donors	0	ACD/ALogP	3.03
Phase 25°C	solid	Rotatable bonds	1	Predicted density	1.4 g/cm ³
SMILES	<chem>O=Cc1c(Cl)cccc1Cl</chem>				
InChIKey	DMYKWPFRFTPY-UHFFFAOYSA-N				

Solubility Data

Solvent	Concentration (M)	Mole Fraction (X)	pph (g/100g)
acetonitrile	1.35	0.08	38.05
chloroform	3.41	0.32	69.35
ethanol	*	*	*
methanol	*	*	*
THF	2.48	0.22	69.58
toluene	1.74	0.19	44.68

* This aldehyde reacts with alcohols to form a hemiacetal.

2,6-dichlorophenylacetic acid C₈H₆Cl₂O₂^{85, 82}



Compound Data

Molecular weight	205.038	H bond acceptors	2	Rule of 5 violations	0
Compound type	carboxylic acid	H bond donors	1	ACD/ALogP	2.71
Phase 25°C	solid	Rotatable bonds	2	Predicted density	1.456 g/cm ³
SMILES	<chem>Clc1cccc(Cl)c1CC(=O)O</chem>				
InChIKey	SFAILOOQFZNOAU-UHFFFAOYSA-N				

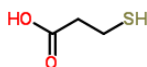
Solubility Data

Solvent	Concentration (M)	Mole Fraction (X)	pph (g/100g)
THF	3.03	0.30	120.05

3-mercaptopropionic acid C₃H₆O₂S²²

Compound Data

Molecular weight	106.144	H bond acceptors	2	Rule of 5 violations	0
Compound type	carboxylic acid	H bond donors	1	ACD/ALogP	0.43

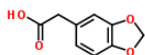


Phase 25°C	liquid	Rotatable bonds	3	Predicted density	1.223 g/cm ³
SMILES	<chem>C(CS)C(=O)O</chem>				
InChIKey	DKIDEFUBRARXTE-UHFFFAOYSA-N				

Solubility Data

Solvent	Concentration (M)	Mole Fraction (X)	pph (g/100g)
methanol	11.48	0.99	44306.20

3,4-(methylenedioxy)phenylacetic acid C₉H₈O₄¹³⁸

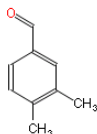


Compound Data					
Molecular weight	180.157	H bond acceptors	4	Rule of 5 violations	0
Compound type	carboxylic acid	H bond donors	1	ACD/ALogP	1.37
Phase 25°C	solid	Rotatable bonds	2	Predicted density	1.406 g/cm ³
SMILES	<chem>O=C(O)Cc1ccc2OCOc2c1</chem>				
InChIKey	ODVLMCWNGKLROU-UHFFFAOYSA-N				

Solubility Data

Solvent	Concentration (M)	Mole Fraction (X)	pph (g/100g)
acetonitrile	0.10	0.01	2.44

3,4-dimethylbenzaldehyde C₉H₁₀O⁵⁹



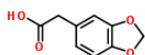
Compound Data					
Molecular weight	134.175	H bond acceptors	1	Rule of 5 violations	0
Compound type	aldehyde	H bond donors	0	ACD/ALogP	2.56
Phase 25°C	liquid	Rotatable bonds	1	Predicted density	1.003 g/cm ³
SMILES	<chem>Cc1ccc(cc1C)C=O</chem>				
InChIKey	POQJHLBMLVTHAU-UHFFFAOYSA-N				

Solubility Data

Solvent	Concentration (M)	Mole Fraction (X)	pph (g/100g)
ethanol	7.54	□	□
methanol	7.54	□	□
THF	7.54	□	□

□ Solute is very soluble/miscible, conversion fail.

3,4-methylenedioxyphenylacetic acid C₉H₈O₄^{129, 132, 131}



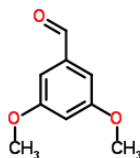
Compound Data					
Molecular weight	180.157	H bond acceptors	4	Rule of 5 violations	0
Compound type	carboxylic acid	H bond donors	1	ACD/ALogP	1.37
Phase 25°C	solid	Rotatable bonds	2	Predicted density	1.406 g/cm ³
SMILES	<chem>O=C(O)Cc1ccc2OCOc2c1</chem>				
InChIKey	ODVLMCWNGKLROU-UHFFFAOYSA-N				

Solubility Data

Solvent	Concentration (M)	Mole Fraction (X)	pph (g/100g)
ethanol	0.55	0.03	13.67
methanol	0.94	0.04	25.57

THF	1.95	0.17	51.81
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3,5-dimethoxybenzaldehyde C₉H₁₀O₃^{205, 208}



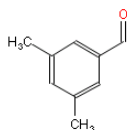
Compound Data

Molecular weight	166.174	H bond acceptors	3	Rule of 5 violations	0
Compound type	aldehyde	H bond donors	0	ACD/ALogP	1.53
Phase 25°C	solid	Rotatable bonds	3	Predicted density	1.114 g/cm ³
SMILES	<chem>O=Cc1cc(OC)cc(OC)c1</chem>				
InChIKey	VFZRZRDOXPRTSC-UHFFFAOYSA-N				

Solubility Data

Solvent	Concentration (M)	Mole Fraction (X)	pph (g/100g)
methanol	1.71	0.09	50.66
THF	4.03	0.45	185.73

3,5-dimethylbenzaldehyde C₉H₁₀O⁶³



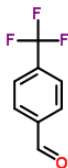
Compound Data

Molecular weight	134.175	H bond acceptors	1	Rule of 5 violations	0
Compound type	aldehyde	H bond donors	0	ACD/ALogP	2.56
Phase 25°C	liquid	Rotatable bonds	1	Predicted density	1.003 g/cm ³
SMILES	<chem>Cc1cc(C=O)cc(C)c1</chem>				
InChIKey	NBEFMISJJNGCIZ-UHFFFAOYSA-N				

Solubility Data

Solvent	Concentration (M)	Mole Fraction (X)	pph (g/100g)
ethanol	7.44	0.99	27092.92
methanol	7.44	0.99	28064.38
THF	7.44	0.99	23376.63

4-(trifluoromethyl)benzaldehyde C₈H₅F₃O²¹



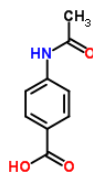
Compound Data

Molecular weight	174.12	H bond acceptors	1	Rule of 5 violations	0
Compound type	aldehyde	H bond donors	0	ACD/ALogP	2.61
Phase 25°C	liquid	Rotatable bonds	1	Predicted density	1.293 g/cm ³
SMILES	<chem>c1cc(C=O)ccc1C(F)(F)F</chem>				
InChIKey	BEOBZEOPTQQELP-UHFFFAOYSA-N				

Solubility Data

Solvent	Concentration (M)	Mole Fraction (X)	pph (g/100g)
methanol	7.32	0.96	11867.65

4-acetamidobenzoic acid C₉H₉NO₃¹³⁷



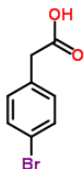
Compound Data

Molecular weight	179.173	H bond acceptors	4	Rule of 5 violations	0
Compound type	carboxylic acid	H bond donors	2	ACD/ALogP	1.31
Phase 25°C	solid	Rotatable bonds	2	Predicted density	1.326 g/cm ³
SMILES	<chem>O=C(Nc1ccc(cc1)C(=O)O)C</chem>				
InChIKey	QCXJEYYXVJIFCE-UHFFFAOYSA-N				

Solubility Data

Solvent	Concentration (M)	Mole Fraction (X)	pph (g/100g)
acetonitrile	0.01	0.00	0.24
benzene	0.00	0.00	0.00
ethanol	0.23	0.01	5.45
methanol	0.19	0.01	4.64
THF	0.17	0.01	3.45

4-bromophenylacetic acid C₈H₇BrO₂⁸⁵



Compound Data

Molecular weight	215.044	H bond acceptors	2	Rule of 5 violations	0
Compound type	carboxylic acid	H bond donors	1	ACD/ALogP	2.28
Phase 25°C	solid	Rotatable bonds	2	Predicted density	1.616 g/cm ³
SMILES	BrC1=CC=C(C=C1)CC(=O)O				
InChIKey	QOWSWEBLNVACCL-UHFFFAOYSA-N				

Solubility Data

Solvent	Concentration (M)	Mole Fraction (X)	pph (g/100g)
THF	3.68	0.37	171.85

4-chloro-3-nitrobenzoic acid C₇H₄ClNO₄^{905, 907}



Compound Data

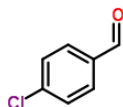
Molecular weight	201.564	H bond acceptors	5	Rule of 5 violations	0
Compound type	carboxylic acid	H bond donors	1	ACD/ALogP	2.37
Phase 25°C	solid	Rotatable bonds	2	Predicted density	1.602 g/cm ³
SMILES	O=[N+](O-)[C@@H]1C=CC(=C1)C(=O)O				
InChIKey	DFXQXFGFOLXAPO-UHFFFAOYSA-N				

Solubility Data

Solvent	Concentration (M)	Mole Fraction (X)	pph (g/100g)
1-butanol	0.31	0.03	8.08
1-decanol	0.19	0.04	4.74
1-heptanol	0.25	0.04	6.34
1-hexanol	0.27	0.03	6.90
1-octanol	0.23	0.04	5.80
1-pentanol	0.27	0.03	6.95
1-propanol	0.37	0.03	9.84
1,4-dioxane	1.43	0.13	35.32
2-butanol	0.32	0.03	8.39
2-ethyl-1-hexanol	0.15	0.02	3.75
2-methyl-1-pentanol	0.19	0.02	4.82
2-methyl-1-propanol	0.19	0.02	4.90
2-methyl-2-propanol	0.38	0.04	10.01
2-pentanol	0.30	0.03	7.77
2-propanol	0.39	0.03	10.45
3-methyl-1-butanol	0.24	0.03	6.17
4-methyl-2-pentanol	0.23	0.03	5.89
butyl acetate	0.23	0.03	5.39
dibutyl ether	0.05	0.01	1.30
diethyl ether	0.24	0.02	6.80
diisopropyl ether	0.10	0.01	2.69
ethanol	0.55	0.03	15.27
ethyl acetate	0.36	0.04	8.46
methyl acetate	0.44	0.04	10.34
methyl butyrate	0.21	0.02	4.88

pentyl acetate	0.16	0.02	3.73
propyl acetate	0.26	0.03	6.08
propylene carbonate	0.15	0.02	2.56
THF	1.95	0.17	57.61
water	0.00	0.00	0.00

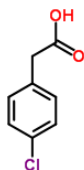
4-chlorobenzaldehyde C₇H₅ClO^{7, 209}



Compound Data			
Molecular weight	140.567	H bond acceptors	1
Compound type	aldehyde	H bond donors	0
Phase 25°C	solid	Rotatable bonds	1
SMILES	O=Cc1ccc(Cl)cc1		
InChIKey	AVPYQKSLYISFPO-UHFFFAOYSA-N		
		Rule of 5 violations	0
		ACD/ALogP	2.21
		Predicted density	1.243 g/cm ³

Solubility Data			
Solvent	Concentration (M)	Mole Fraction (X)	pph (g/100g)
acetonitrile	5.58	0.45	285.27
chloroform	3.61	0.33	57.17
ethanol	2.81	0.20	74.23
methanol	3.55	0.20	110.72
THF	5.29	0.51	204.25

4-chlorophenylacetic acid C₈H₇ClO₂^{4, 75, 73}

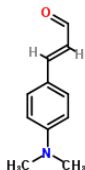


Compound Data			
Molecular weight	170.593	H bond acceptors	2
Compound type	carboxylic acid	H bond donors	1
Phase 25°C	solid	Rotatable bonds	2
SMILES	Clc1ccc(cc1)CC(=O)O		
InChIKey	CDPKJZJVTHSESZ-UHFFFAOYSA-N		
		Rule of 5 violations	0
		ACD/ALogP	2.1
		Predicted density	1.324 g/cm ³

Solubility Data			
Solvent	Concentration (M)	Mole Fraction (X)	pph (g/100g)
acetonitrile	1.67	0.10	48.72
DMSO	5.74	0.61	342.14
methanol	7.76	□	□
THF	4.45	0.45	197.18
toluene	0.89	0.10	19.69

□ Solute is very soluble/miscible, conversion fail.

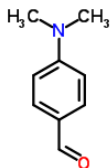
4-dimethylamino cinnamaldehyde C₁₁H₁₃NO^{3, 32}



Compound Data			
Molecular weight	175.227	H bond acceptors	2
Compound type	aldehyde	H bond donors	0
Phase 25°C	solid	Rotatable bonds	3
SMILES	O=CC=Cc1ccc(N(C)C)cc1		
InChIKey	RUKJCCJILIMGEP-ONEGZZNKSA-N		
		Rule of 5 violations	0
		ACD/ALogP	2.63
		Predicted density	1.057 g/cm ³

Solubility Data			
Solvent	Concentration (M)	Mole Fraction (X)	pph (g/100g)
ethanol	0.06	0.00	1.25
methanol	0.07	0.00	1.65
THF	0.42	0.03	8.75

4-dimethylaminobenzaldehyde C₉H₁₁NO^{208, 205}



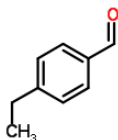
Compound Data

Molecular weight	149.19	H bond acceptors	2	Rule of 5 violations	0
Compound type	aldehyde	H bond donors	0	ACD/ALogP	1.81
Phase 25°C	solid	Rotatable bonds	2	Predicted density	1.072 g/cm ³
SMILES	<chem>O=Cc1ccc(N(C)C)cc1</chem>				
InChIKey	BGNGWHSBYQYVRX-UHFFFAOYSA-N				

Solubility Data

Solvent	Concentration (M)	Mole Fraction (X)	pph (g/100g)
acetonitrile	2.60	0.18	81.37
chloroform	4.02	0.42	90.76
ethanol	0.63	0.04	13.21
methanol	1.36	0.07	33.24
THF	2.50	0.23	63.27
toluene	1.54	0.17	33.57

4-ethylbenzaldehyde C₉H₁₀O⁶³



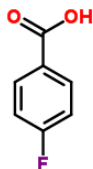
Compound Data

Molecular weight	134.175	H bond acceptors	1	Rule of 5 violations	0
Compound type	aldehyde	H bond donors	0	ACD/ALogP	2.63
Phase 25°C	liquid	Rotatable bonds	2	Predicted density	1.001 g/cm ³
SMILES	<chem>CCc1ccc(C=O)cc1</chem>				
InChIKey	QNGNSVIICDLXHT-UHFFFAOYSA-N				

Solubility Data

Solvent	Concentration (M)	Mole Fraction (X)	pph (g/100g)
ethanol	7.30	0.95	5840.38
methanol	7.30	0.94	6049.80
THF	7.30	0.96	5039.27

4-fluorobenzoic acid C₇H₅FO₂^{106, 121, 907}



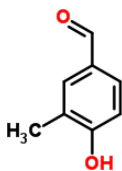
Compound Data

Molecular weight	140.112	H bond acceptors	2	Rule of 5 violations	0
Compound type	carboxylic acid	H bond donors	1	ACD/ALogP	2.07
Phase 25°C	solid	Rotatable bonds	1	Predicted density	1.319 g/cm ³
SMILES	<chem>O=C(O)c1ccc(F)cc1</chem>				
InChIKey	BBYDXOIZLAWGSL-UHFFFAOYSA-N				

Solubility Data

Solvent	Concentration (M)	Mole Fraction (X)	pph (g/100g)
acetonitrile	0.39	0.02	7.63
DMSO	4.19	0.35	96.26
ethanol	0.80	0.05	15.71
methanol	0.76	0.03	15.38
THF	2.49	0.21	52.47
toluene	0.00	0.00	0.00
water	0.01	0.00	0.14

4-hydroxy-3-methylbenzaldehyde C₈H₈O₂⁵⁷



Compound Data

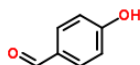
Molecular weight	136.148	H bond acceptors	2	Rule of 5 violations	0
Compound type	aldehyde	H bond donors	1	ACD/ALogP	1.85
Phase 25°C	solid	Rotatable bonds	2	Predicted density	1.175 g/cm ³
SMILES	<chem>O=Cc1ccc(O)c(c1)C</chem>				
InChIKey	BAKYASSDAXQKKY-UHFFFAOYSA-N				

Solubility Data

Solvent	Concentration (M)	Mole Fraction (X)	pph (g/100g)
ethanol	2.15	0.14	49.98
methanol	2.78	0.15	74.15
THF	3.05	0.27	71.04

4-hydroxybenzaldehyde C₇H₆O₂^{208, 57, 205, 58, 88, 85, 909}

Compound Data

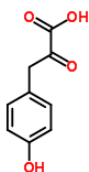


Molecular weight	122.121	H bond acceptors	2	Rule of 5 violations	0
Compound type	aldehyde	H bond donors	1	ACD/ALogP	1.39
Phase 25°C	solid	Rotatable bonds	2	Predicted density	1.226 g/cm ³
SMILES	<chem>O=Cc1ccc(O)cc1</chem>				
InChIKey	RGHHSNMVTDWUBI-UHFFFAOYSA-N				

Solubility Data

Solvent	Concentration (M)	Mole Fraction (X)	pph (g/100g)
acetonitrile	1.46	0.09	27.93
chloroform	1.75	0.14	17.26
ethanol	2.52	0.17	52.82
methanol	3.39	0.18	83.19
THF	3.70	0.32	79.10
toluene	0.02	0.00	0.28
water	0.11	0.00	1.36

4-hydroxyphenylpyruvic acid C₉H₈O₄¹⁵



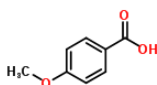
Compound Data

Molecular weight	180.157	H bond acceptors	4	Rule of 5 violations	0
Compound type	carboxylic acid	H bond donors	2	ACD/ALogP	-0.2
Phase 25°C	solid	Rotatable bonds	4	Predicted density	1.397 g/cm ³
SMILES	<chem>c1cc(O)ccc1CC(=O)C(=O)O</chem>				
InChIKey	KKADPXVIOXHVKI-UHFFFAOYSA-N				

Solubility Data

Solvent	Concentration (M)	Mole Fraction (X)	pph (g/100g)
ethanol	0.71	0.04	18.05
methanol	0.91	0.04	24.67

4-methoxybenzoic acid C₈H₈O₃⁹⁰⁵



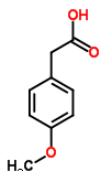
Compound Data

Molecular weight	152.147	H bond acceptors	3	Rule of 5 violations	0
Compound type	carboxylic acid	H bond donors	1	ACD/ALogP	1.96
Phase 25°C	solid	Rotatable bonds	2	Predicted density	1.207 g/cm ³
SMILES	<chem>COc1ccc(cc1)C(=O)O</chem>				
InChIKey	ZEYHEAKUIGZSGI-UHFFFAOYSA-N				

Solubility Data

Solvent	Concentration (M)	Mole Fraction (X)	pph (g/100g)
1-butanol	0.12	0.01	2.30
1-decanol	0.07	0.01	1.30
1-heptanol	0.09	0.01	1.69
1-hexanol	0.10	0.01	1.89
1-octanol	0.08	0.01	1.49
1-pentanol	0.10	0.01	1.90
1-propanol	0.13	0.01	2.53
1,4-dioxane	0.39	0.04	6.27
2-butanol	0.13	0.01	2.51
2-ethyl-1-hexanol	0.07	0.01	1.31
2-methyl-1-propanol	0.08	0.01	1.54
2-methyl-2-propanol	0.17	0.02	3.29
2-propanol	0.14	0.01	2.74
3-methyl-1-butanol	0.08	0.01	1.52
butyl acetate	0.08	0.01	1.39
dibutyl ether	0.02	0.00	0.39
diethyl ether	0.09	0.01	1.89
diisopropyl ether	0.03	0.00	0.60
ethanol	0.20	0.01	4.00
ethyl acetate	0.13	0.01	2.24
pentyl acetate	0.06	0.01	1.04
THF	0.70	0.06	12.92

4-methoxyphenylacetic acid C₉H₁₀O₃^{89, 136, 92, 910}



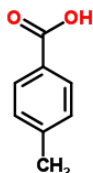
Compound Data

Molecular weight	166.174	H bond acceptors	3	Rule of 5 violations	0
Compound type	carboxylic acid	H bond donors	1	ACD/ALogP	1.42
Phase 25°C	solid	Rotatable bonds	3	Predicted density	1.179 g/cm ³
SMILES	<chem>O=C(O)Cc1ccc(OC)cc1</chem>				
InChIKey	NRPFNQUDKRYCNX-UHFFFAOYSA-N				

Solubility Data

Solvent	Concentration (M)	Mole Fraction (X)	pph (g/100g)
acetonitrile	2.23	0.15	72.11
DMSO	4.50	0.47	186.41
methanol	2.50	0.14	85.19
THF	3.31	0.33	114.38
toluene	0.37	0.04	7.45
water	0.04	0.00	0.67

4-methylbenzoic acid C₈H₈O₂^{2, 25}



Compound Data

Molecular weight	136.148	H bond acceptors	2	Rule of 5 violations	0
Compound type	carboxylic acid	H bond donors	1	ACD/ALogP	2.36
Phase 25°C	solid	Rotatable bonds	1	Predicted density	1.151 g/cm ³
SMILES	<chem>O=C(O)c1ccc(C)cc1</chem>				
InChIKey	LPNBBFKOUUSUDB-UHFFFAOYSA-N				

Solubility Data

Solvent	Concentration (M)	Mole Fraction (X)	pph (g/100g)
ethanol	0.78	0.05	14.89
methanol	0.78	0.04	15.54

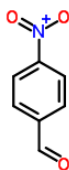
THF

1.60

0.14

29.84

4-nitrobenzaldehyde C₇H₅NO₃^{904, 111, 98, 212, 33, 205, 82, 122}



Compound Data

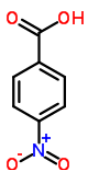
Molecular weight	151.12	H bond acceptors	4	Rule of 5 violations	0
Compound type	aldehyde	H bond donors	0	ACD/ALogP	1.56
Phase 25°C	solid	Rotatable bonds	2	Predicted density	1.338 g/cm ³
SMILES	<chem>c1cc(C=O)ccc1[N+](=O)[O-]</chem>				
InChIKey	BXRFQSNORATLV-UHFFFAOYSA-N				

Solubility Data

Solvent	Concentration (M)	Mole Fraction (X)	pph (g/100g)
1-butanol	*	*	*
1-propanol	*	*	*
2-propanol	*	*	*
acetonitrile	1.13	0.07	26.16
benzene	0.46	0.04	8.40
carbon tetrachloride	0.07	0.01	0.63
chloroform	1.02	0.08	11.57
cyclohexane	0.01	0.00	0.19
dichloromethane	1.29	0.09	18.23
DMF	1.68	0.15	36.02
DMSO	1.24	0.09	19.83
ethanol	*	*	*
ethylene glycol	*	*	*
methanol	*	*	*
THF	0.88	0.07	16.33
toluene	0.46	0.05	8.42

* This aldehyde reacts with alcohols to form a hemiacetal.

4-nitrobenzoic acid C₇H₅NO₄⁹⁰⁵



Compound Data

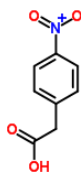
Molecular weight	167.119	H bond acceptors	5	Rule of 5 violations	0
Compound type	carboxylic acid	H bond donors	1	ACD/ALogP	1.89
Phase 25°C	solid	Rotatable bonds	2	Predicted density	1.468 g/cm ³
SMILES	<chem>O=[N+]([O-])c1ccc(C(=O)O)cc1</chem>				
InChIKey	OTLNPYWUJOZPPA-UHFFFAOYSA-N				

Solubility Data

Solvent	Concentration (M)	Mole Fraction (X)	pph (g/100g)
1-butanol	0.09	0.01	1.89
1-decanol	0.05	0.01	1.01
1-heptanol	0.08	0.01	1.65
1-hexanol	0.08	0.01	1.65
1-octanol	0.06	0.01	1.23
1-pentanol	0.09	0.01	1.87
1-propanol	0.11	0.01	2.34
1,4-dioxane	0.47	0.04	8.34
2-butanol	0.10	0.01	2.11
2-methyl-1-butanol	0.05	0.01	1.04
2-methyl-1-pentanol	0.05	0.01	1.03
2-methyl-1-propanol	0.07	0.01	1.47
2-methyl-2-butanol	0.17	0.02	3.57
2-methyl-2-propanol	0.15	0.01	3.17
2-pentanol	0.08	0.01	1.67
2-propanol	0.11	0.01	2.35

3-methyl-1-butanol	0.07	0.01	1.46
4-methyl-2-pentanol	0.07	0.01	1.45
butyl acetate	0.08	0.01	1.52
dibutyl ether	0.02	0.00	0.43
diethyl ether	0.10	0.01	2.30
diisopropyl ether	0.03	0.00	0.66
ethanol	0.14	0.01	3.05
ethyl acetate	0.13	0.01	2.46
methanol	0.18	0.01	4.08
methyl acetate	0.14	0.01	2.62
pentyl acetate	0.05	0.01	0.95
propylene carbonate	0.06	0.01	0.84
THF	0.78	0.06	15.82

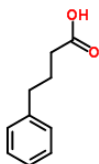
4-nitrophenylacetic acid C₈H₇NO₄¹⁵



Compound Data			
Molecular weight	181.145	H bond acceptors	5 Rule of 5 violations 0
Compound type	carboxylic acid	H bond donors	1 ACD/ALogP 1.24
Phase 25°C	solid	Rotatable bonds	3 Predicted density 1.407 g/cm ³
SMILES	c1cc(CC(=O)O)ccc1[N+](=O)[O-]		
InChIKey	YBADLXQNJCMBKR-UHFFFAOYSA-N		

Solubility Data			
Solvent	Concentration (M)	Mole Fraction (X)	pph (g/100g)
ethanol	0.71	0.04	18.15
methanol	1.29	0.06	37.21

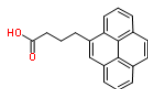
4-phenylbutyric acid C₁₀H₁₂O₂⁷²



Compound Data			
Molecular weight	164.201	H bond acceptors	2 Rule of 5 violations 0
Compound type	carboxylic acid	H bond donors	1 ACD/ALogP 2.42
Phase 25°C	solid	Rotatable bonds	4 Predicted density 1.095 g/cm ³
SMILES	O=C(O)CCCc1ccccc1		
InChIKey	OBKXEAXTFZPCHS-UHFFFAOYSA-N		

Solubility Data			
Solvent	Concentration (M)	Mole Fraction (X)	pph (g/100g)
1-hexanol	0.19	0.02	3.94
chloroform	3.99	0.44	108.74
diethyl ether	4.02	0.51	226.42
methanol	4.54	0.38	310.15
toluene	4.06	0.52	195.66

4-pyrenebutanoic acid C₂₀H₁₆O₂^{61, 99, 51, 30, 24, 91, 84}



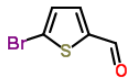
Compound Data			
Molecular weight	288.34	H bond acceptors	2 Rule of 5 violations 1
Compound type	carboxylic acid	H bond donors	1 ACD/ALogP 5.37
Phase 25°C	solid	Rotatable bonds	4 Predicted density 1.296 g/cm ³
SMILES	O=C(O)CCC4cc2cccc1ccc3c(c12)c4ccc3		
InChIKey	GSBSDUZVSCTUKA-UHFFFAOYSA-N		

Solubility Data			
Solvent	Concentration	Mole Fraction (X)	pph (g/100g)

	(M)		
2-propanol	0.06	0.00	2.22
acetonitrile	0.00	0.00	0.00
benzene	0.00	0.00	0.00
carbon tetrachloride	0.00	0.00	0.00
chloroform	0.03	0.00	0.58
cyclohexane	0.00	0.00	0.00
cyclopentane	0.00	0.00	0.00
dichloromethane	0.07	0.00	1.64
diethyl ether	0.02	0.00	0.79
DMF	1.88	0.21	107.11
DMSO	2.07	0.21	100.37
ethanol	0.06	0.00	2.25
hexane	0.00	0.00	0.00
methanol	0.01	0.00	0.51
THF	0.55	0.05	19.99
toluene	0.00	0.00	0.00

5-bromothiophene-2-carbaldehyde C₅H₃BrOS²¹

Compound Data

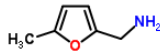
	Molecular weight	191.046	H bond acceptors	1	Rule of 5 violations	0
	Compound type	aldehyde	H bond donors	0	ACD/ALogP	1.97
	Phase 25°C	liquid	Rotatable bonds	1	Predicted density	1.789 g/cm ³
	SMILES	C1=C(SC(=C1)Br)C=O				
	InChIKey	GFBVUFQNHLCUPX-UHFFFAOYSA-N				

Solubility Data

Solvent	Concentration (M)	Mole Fraction (X)	pph (g/100g)
methanol	9.22	0.96	15186.93

5-methylfurfurylamine C₆H₉NO²⁶

Compound Data

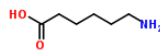
	Molecular weight	111.142	H bond acceptors	2	Rule of 5 violations	0
	Compound type	amine	H bond donors	2	ACD/ALogP	0.71
	Phase 25°C	liquid	Rotatable bonds	2	Predicted density	1.024 g/cm ³
	SMILES	Cc1cc(CCN)oc1				
	InChIKey	YSEAGSCGERFGBL-UHFFFAOYSA-N				

Solubility Data

Solvent	Concentration (M)	Mole Fraction (X)	pph (g/100g)
methanol	8.97	0.94	5010.81

6-aminocaproic acid C₆H₁₃NO₂¹⁴

Compound Data

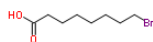
	Molecular weight	131.173	H bond acceptors	3	Rule of 5 violations	0
	Compound type	carboxylic acid	H bond donors	3	ACD/ALogP	-0.11
	Phase 25°C	solid	Rotatable bonds	6	Predicted density	1.042 g/cm ³
	SMILES	C(CCC(=O)O)CCN				
	InChIKey	SLXKOJJOQWFEFD-UHFFFAOYSA-N				

Solubility Data

Solvent	Concentration (M)	Mole Fraction (X)	pph (g/100g)
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ethanol	0.00	0.00	0.00
methanol	0.06	0.00	1.05

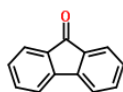
8-bromooctanoic acid C₈H₁₅BrO₂^{3, 66}



Compound Data			
Molecular weight	223.107	H bond acceptors	2 Rule of 5 violations 0
Compound type	carboxylic acid	H bond donors	1 ACD/ALogP 2.76
Phase 25°C	solid	Rotatable bonds	7 Predicted density 1.324 g/cm ³
SMILES	BrCCCCCCCC(=O)O		
InChIKey	BKJFDZSBZWHRNH-UHFFFAOYSA-N		

Solubility Data			
Solvent	Concentration (M)	Mole Fraction (X)	pph (g/100g)
ethanol	4.07	0.43	370.56
methanol	3.28	0.24	217.27
THF	3.56	0.42	219.59

9-fluorenone C₁₃H₈O⁹⁰⁵

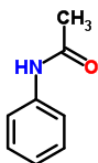


Compound Data			
Molecular weight	180.202	H bond acceptors	1 Rule of 5 violations 0
Compound type	non-Ugi related	H bond donors	0 ACD/ALogP 3.58
Phase 25°C	solid	Rotatable bonds	0 Predicted density 1.244 g/cm ³
SMILES	O=C3c1ccccc1c2c3ccccc2		
InChIKey	YLQWCDOJCJODRMT-UHFFFAOYSA-N		

Solubility Data			
Solvent	Concentration (M)	Mole Fraction (X)	pph (g/100g)
1-butanol	0.37	0.03	8.75
1-decanol	0.42	0.08	9.73
1-heptanol	0.43	0.06	10.08
1-hexanol	0.41	0.05	9.63
1-octanol	0.43	0.07	10.04
1-pentanol	0.41	0.05	9.69
1-propanol	0.38	0.03	9.12
2-butanol	0.33	0.03	7.80
2-ethyl-1-hexanol	0.35	0.06	8.09
2-methyl-1-pentanol	0.36	0.05	8.41
2-methyl-1-propanol	0.25	0.02	5.84
2-methyl-2-butanol	0.40	0.04	9.43
2-methyl-2-propanol	0.31	0.03	7.27
2-pentanol	0.35	0.04	8.21
2-propanol	0.29	0.02	6.90
2,2,4-trimethylpentane	0.07	0.01	1.80
3-methyl-1-butanol	0.31	0.03	7.23
4-methyl-2-pentanol	0.29	0.04	6.73
acetonitrile	1.57	0.10	49.02
benzene	2.61	0.27	86.63
butyronitrile	1.93	0.19	61.50
carbon tetrachloride	1.83	0.18	26.44
cyclohexane	0.15	0.02	3.50
cyclooctane	0.17	0.02	3.98
cyclopentanol	0.82	0.07	16.70
decane	0.12	0.02	3.00
dibutyl ether	0.37	0.06	9.03
dichloromethane	4.03	0.40	139.36
diethyl ether	0.88	0.09	24.76

diisopropyl ether	0.37	0.05	9.29
ethanol	3.08	0.25	128.48
heptane	0.11	0.02	2.90
hexadecane	0.12	0.03	2.85
hexane	0.10	0.01	2.71
methanol	0.37	0.02	9.36
methyl tert-butyl ether	0.76	0.09	20.52
methylcyclohexane	0.14	0.02	3.32
nonane	0.12	0.02	3.04
octane	0.11	0.02	2.83
propionitrile	1.99	0.17	65.35
tert-butylcyclohexane	0.12	0.02	2.71
toluene	2.17	0.25	65.48
undecane	0.12	0.03	2.96

acetanilide C₈H₉NO³⁵



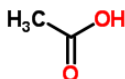
Compound Data

Molecular weight	135.163	H bond acceptors	2	Rule of 5 violations	0
Compound type	amide	H bond donors	1	ACD/ALogP	1.08
Phase 25°C	solid	Rotatable bonds	1	Predicted density	1.103 g/cm ³
SMILES	O=C(Nc1ccccc1)C				
InChIKey	FZERIULMFGESH-UHFFFAOYSA-N				

Solubility Data

Solvent	Concentration (M)	Mole Fraction (X)	pph (g/100g)
acetone	1.42	0.11	30.10

acetic acid C₂H₄O₂²²



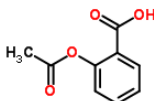
Compound Data

Molecular weight	60.052	H bond acceptors	2	Rule of 5 violations	0
Compound type	carboxylic acid	H bond donors	1	ACD/ALogP	-0.29
Phase 25°C	liquid	Rotatable bonds	0	Predicted density	1.068 g/cm ³
SMILES	O=C(O)C				
InChIKey	QTBSBXVTEAMEQO-UHFFFAOYSA-N				

Solubility Data

Solvent	Concentration (M)	Mole Fraction (X)	pph (g/100g)
methanol	17.47	0.98	7876.42

acetylsalicylic acid C₉H₈O₄^{72, 34, 903, 907}



Compound Data

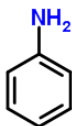
Molecular weight	180.157	H bond acceptors	4	Rule of 5 violations	0
Compound type	carboxylic acid	H bond donors	1	ACD/ALogP	1.19
Phase 25°C	solid	Rotatable bonds	3	Predicted density	1.29 g/cm ³
SMILES	O=C(Oc1ccccc1C(=O)O)C				
InChIKey	BSYNRYMUTXBXSQ-UHFFFAOYSA-N				

Solubility Data

Solvent	Concentration (M)	Mole Fraction (X)	pph (g/100g)
1-hexanol	0.00	0.00	0.00
chloroform	0.18	0.01	2.24
diethyl ether	0.17	0.02	4.27

methanol	1.30	0.06	38.00
toluene	0.00	0.00	0.00
water	0.03	0.00	0.45

aniline C₆H₇N²⁹



Compound Data

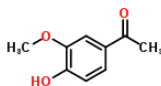
Molecular weight	93.1265	H bond acceptors	1	Rule of 5 violations	0
Compound type	amine	H bond donors	2	ACD/ALogP	0.94
Phase 25°C	liquid	Rotatable bonds	1	Predicted density	1.015 g/cm ³
SMILES	Nc1ccccc1				
InChIKey	PAYRUJLWNCNPSJ-UHFFFAOYSA-N				

Solubility Data

Solvent	Concentration (M)	Mole Fraction (X)	pph (g/100g)
methanol	10.97	□	□

□ Solute is very soluble/miscible, conversion fail.

apocynin C₉H₁₀O₃⁹⁰⁶



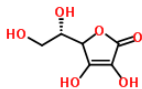
Compound Data

Molecular weight	166.174	H bond acceptors	3	Rule of 5 violations	0
Compound type	non-Ugi related	H bond donors	1	ACD/ALogP	1.39
Phase 25°C	solid	Rotatable bonds	3	Predicted density	1.158 g/cm ³
SMILES	Oc1ccc(cc1OC)C(C)=O				
InChIKey	DFYRUELUNQRZTB-UHFFFAOYSA-N				

Solubility Data

Solvent	Concentration (M)	Mole Fraction (X)	pph (g/100g)
1-propanol	0.32	0.02	7.01
1,2-dichloroethane	0.41	0.04	6.17
butanone	0.66	0.06	15.41
toluene	0.06	0.01	1.15

ascorbic acid C₉H₈O₄⁷²



Compound Data

Molecular weight	180.157	H bond acceptors	4	Rule of 5 violations	0
Compound type	carboxylic acid	H bond donors	1	ACD/ALogP	1.19
Phase 25°C	solid	Rotatable bonds	3	Predicted density	1.29 g/cm ³
SMILES	O=C1=C(/O)C(=O)O[C@@H]1[C@@H](O)CO				
InChIKey	CIWBSHSKHKDKBQ-JLAZNSOCSA-N				

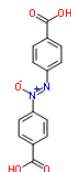
Solubility Data

Solvent	Concentration (M)	Mole Fraction (X)	pph (g/100g)
1-hexanol	0.00	0.00	0.00
chloroform	0.00	0.00	0.00
diethyl ether	0.00	0.00	0.00
toluene	0.00	0.00	0.00

azoxydibenzoic acid C₁₄H₁₀N₂O₅⁷²

Compound Data

Molecular weight	286.24	H bond acceptors	7	Rule of 5 violations	0
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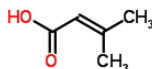


Compound type	carboxylic acid	H bond donors	2	ACD/ALogP	4.05
Phase 25°C	solid	Rotatable bonds	4	Predicted density	1.41 g/cm ³
SMILES	<chem>O=C(O)c2ccc([N+](=O-)=N/c1ccc(cc1)C(=O)O)cc2</chem>				
InChIKey	ZYVHVJGJGLOEEKD-NXVVXOECSA-N				

Solubility Data

Solvent	Concentration (M)	Mole Fraction (X)	pph (g/100g)
1-hexanol	0.00	0.00	0.00
chloroform	0.00	0.00	0.00
diethyl ether	0.00	0.00	0.00
toluene	0.00	0.00	0.00

B,B-dimethylacrylic acid C₅H₈O₂¹³⁶

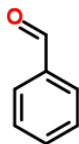


Molecular weight	100.116	H bond acceptors	2	Rule of 5 violations	0
Compound type	carboxylic acid	H bond donors	1	ACD/ALogP	1.35
Phase 25°C	solid	Rotatable bonds	1	Predicted density	1.01 g/cm ³
SMILES	<chem>O=C(O)C=C(C)C</chem>				
InChIKey	YYPNJNDODFVZLE-UHFFFAOYSA-N				

Solubility Data

Solvent	Concentration (M)	Mole Fraction (X)	pph (g/100g)
methanol	4.73	0.27	118.40

benzaldehyde C₇H₆O²¹

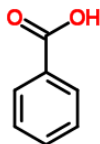


Molecular weight	106.122	H bond acceptors	1	Rule of 5 violations	0
Compound type	aldehyde	H bond donors	0	ACD/ALogP	1.64
Phase 25°C	liquid	Rotatable bonds	1	Predicted density	1.049 g/cm ³
SMILES	<chem>c1ccccc1C=O</chem>				
InChIKey	HUMNYLRZRPJDN-UHFFFAOYSA-N				

Solubility Data

Solvent	Concentration (M)	Mole Fraction (X)	pph (g/100g)
methanol	9.85	0.99	39374.95

benzoic acid C₇H₆O₂^{155, 37, 902, 58, 160, 43, 136, 9, 907, 900}



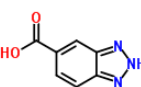
Molecular weight	122.121	H bond acceptors	2	Rule of 5 violations	0
Compound type	carboxylic acid	H bond donors	1	ACD/ALogP	1.9
Phase 25°C	solid	Rotatable bonds	1	Predicted density	1.197 g/cm ³
SMILES	<chem>O=C(O)c1ccccc1</chem>				
InChIKey	WPYMKLBDIGXBTP-UHFFFAOYSA-N				

Solubility Data

Solvent	Concentration (M)	Mole Fraction (X)	pph (g/100g)
1-octanol	1.48	0.22	25.97
acetone	1.35	0.11	24.77

acetonitrile	0.75	0.04	13.37
benzene	0.48	0.04	7.06
chloroform	1.80	0.15	17.95
ethanol	2.55	0.17	54.02
methanol	2.84	0.15	64.81
THF	3.37	0.29	69.27
toluene	0.65	0.07	9.81
water	0.03	0.00	0.36

benzotriazole-5-carboxylic acid $C_7H_5N_3O_2$ ^{3, 32}

	Compound Data			
	Molecular weight	163.133	H bond acceptors	5 Rule of 5 violations 0
	Compound type	carboxylic acid	H bond donors	2 ACD/ALogP 0.82
	Phase 25°C	solid	Rotatable bonds	1 Predicted density 1.617 g/cm ³
	SMILES	O=C(O)c1ccc2nnnc2c1		
	InChIKey			

Solubility Data			
Solvent	Concentration (M)	Mole Fraction (X)	pph (g/100g)
ethanol	0.04	0.00	0.73
methanol	0.04	0.00	0.76
THF	0.02	0.00	0.36

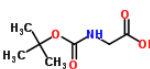
benzylamine C_7H_9N ²⁹

	Compound Data			
	Molecular weight	107.153	H bond acceptors	1 Rule of 5 violations 0
	Compound type	amine	H bond donors	2 ACD/ALogP 1.09
	Phase 25°C	liquid	Rotatable bonds	2 Predicted density 0.979 g/cm ³
	SMILES	NCc1ccccc1		
	InChIKey	WGQKYBSKWIADBV-UHFFFAOYSA-N		

Solubility Data			
Solvent	Concentration (M)	Mole Fraction (X)	pph (g/100g)
methanol	9.16	□	□

□ Solute is very soluble/miscible, conversion fail.

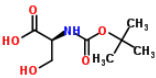
boc-glycine $C_7H_{13}NO_4$ ^{143, 71, 207, 135, 133, 116}

	Compound Data				
	Molecular weight	175.182	H bond acceptors	5 Rule of 5 violations	0
	Compound type	carboxylic acid	H bond donors	2 ACD/ALogP	0.75
	Phase 25°C	solid	Rotatable bonds	4 Predicted density	1.159 g/cm ³
	SMILES	O=C(OC(C)(C)C)NCC(=O)O			
	InChIKey	VRPJIFMKZZEXLR-UHFFFAOYSA-N			

Solubility Data			
Solvent	Concentration (M)	Mole Fraction (X)	pph (g/100g)
2-propanol	3.63	0.38	177.58
acetonitrile	2.46	0.18	91.84
benzene	0.25	0.02	5.32
chloroform	3.85	0.42	107.55
dichloromethane	4.14	0.43	154.79
diethyl ether	2.65	0.31	105.51

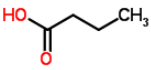
DMSO	4.78	0.55	274.57
ethanol	4.11	0.39	243.70
hexane	0.25	0.03	6.74
methanol	4.72	0.41	384.60
THF	3.72	0.40	164.41
toluene	0.19	0.02	3.93

boc-serine C₈H₁₅NO₅^{98, 85}

Compound Data			
	Molecular weight 205.208	H bond acceptors 6	Rule of 5 violations 0
	Compound type boc serine	H bond donors 3	ACD/ALogP 0.22
	Phase 25°C solid	Rotatable bonds 6	Predicted density 1.24 g/cm ³
	SMILES O=C(OC(C)(C)C)N[C@H](C(=O)O)CO		
	InChIKey FHOAKXBXYJSJBGX-YFKPBYRVSA-N		

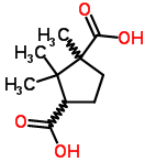
Solubility Data			
Solvent	Concentration (M)	Mole Fraction (X)	pph (g/100g)
methanol	3.62	0.28	246.06
THF	3.11	0.34	145.78

butyric acid C₄H₈O₂²²

Compound Data			
	Molecular weight 88.1051	H bond acceptors 2	Rule of 5 violations 0
	Compound type carboxylic acid	H bond donors 1	ACD/ALogP 0.78
	Phase 25°C liquid	Rotatable bonds 2	Predicted density 0.987 g/cm ³
	SMILES CCCC(=O)O		
	InChIKey FERIUCNNQQJTOY-UHFFFAOYSA-N		

Solubility Data			
Solvent	Concentration (M)	Mole Fraction (X)	pph (g/100g)
methanol	10.94	0.95	5462.12

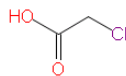
camphoric acid C₁₀H₁₆O₄⁹⁰²

Compound Data			
	Molecular weight 200.232	H bond acceptors 4	Rule of 5 violations 0
	Compound type carboxylic acid	H bond donors 2	ACD/ALogP 1.47
	Phase 25°C solid	Rotatable bonds 2	Predicted density 1.177 g/cm ³
	SMILES O=C(O)C1CCC(C(=O)O)(C)C1(C)C		
	InChIKey LSPHULWDVZXLIL-UHFFFAOYSA-N		

Solubility Data			
Solvent	Concentration (M)	Mole Fraction (X)	pph (g/100g)
1-propanol	1.72	0.16	61.24
methanol	2.75	0.18	137.41

chloroacetic acid C₂H₃ClO₂⁹⁵

Compound Data			
Molecular weight 94.497	H bond acceptors 2	Rule of 5 violations 0	
Compound type carboxylic acid	H bond donors 1	ACD/ALogP 0.18	
Phase 25°C solid	Rotatable bonds 1	Predicted density 1.398 g/cm ³	

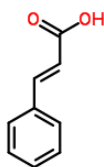


SMILES ClCC(=O)O
InChIKey FOCAUTSVDIKZOP-UHFFFAOYSA-N

Solubility Data

Solvent	Concentration (M)	Mole Fraction (X)	pph (g/100g)
acetonitrile	12.45	0.81	993.98
DMSO	11.20	0.77	396.40
methanol	9.45	0.53	328.30
THF	9.63	0.69	288.10
toluene	1.41	0.14	16.95

cinnamic acid $C_9H_8O_2$ ^{72, 902, 48, 907}



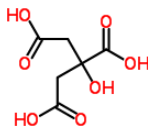
Compound Data

Molecular weight 148.159 **H bond acceptors** 2 **Rule of 5 violations** 0
Compound type carboxylic acid **H bond donors** 1 **ACD/ALogP** 2.38
Phase 25°C solid **Rotatable bonds** 2 **Predicted density** 1.184 g/cm³
SMILES O=C(O)C=Cc1ccccc1
InChIKey WBYWAXJHAXSJNI-VOTSOKGWSA-N

Solubility Data

Solvent	Concentration (M)	Mole Fraction (X)	pph (g/100g)
1-hexanol	0.00	0.00	0.00
chloroform	0.93	0.08	10.40
diethyl ether	0.43	0.04	9.17
ethanol	0.86	0.05	18.31
methanol	1.10	0.05	25.19
toluene	0.30	0.03	5.30
water	0.00	0.00	0.00

citric acid anhydrous $C_6H_8O_7$ ^{902, 25}



Compound Data

Molecular weight 192.124 **H bond acceptors** 7 **Rule of 5 violations** 0
Compound type carboxylic acid **H bond donors** 4 **ACD/ALogP** -1.33
Phase 25°C solid **Rotatable bonds** 6 **Predicted density** 1.762 g/cm³
SMILES O=C(O)CC(O)(C(=O)O)CC(=O)O
InChIKey KRKNYBCHXYNGOX-UHFFFAOYSA-N

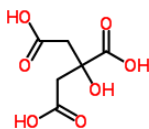
Solubility Data

Solvent	Concentration (M)	Mole Fraction (X)	pph (g/100g)
chloroform	0.00	0.00	0.00
ethanol	1.60	0.10	47.74
methanol	3.08	0.16	118.32
THF	1.80	0.15	47.60

citric acid monohydrate $C_6H_8O_7 \cdot 2$

Compound Data

Molecular weight 192.124 **H bond acceptors** 7 **Rule of 5 violations** 0
Compound type carboxylic acid **H bond donors** 4 **ACD/ALogP** -1.33

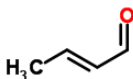


Phase 25°C	solid	Rotatable bonds	6	Predicted density	1.762 g/cm ³
SMILES	<chem>O=C(O)CC(O)(C(=O)O)CC(=O)O</chem>				
InChIKey	KRKNYBCHXYNGOX-UHFFFAOYSA-N				

Solubility Data

Solvent	Concentration (M)	Mole Fraction (X)	pph (g/100g)
ethanol	1.78	0.12	54.40
methanol	2.27	0.11	76.97
THF	1.52	0.13	38.72

crotonaldehyde C₄H₆O²¹



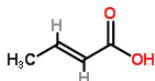
Molecular weight	70.0898	H bond acceptors	1	Rule of 5 violations	0
Compound type	aldehyde	H bond donors	0	ACD/ALogP	0.88
Phase 25°C	solid	Rotatable bonds	1	Predicted density	0.819 g/cm ³
SMILES	<chem>CC=CC=O</chem>				
InChIKey	MLUCVPSAIODCQM-NSCUHMNNSA-N				

Solubility Data

Solvent	Concentration (M)	Mole Fraction (X)	pph (g/100g)
methanol	12.17	□	□

□ Solute is very soluble/miscible, conversion fail.

crotonic acid C₄H₆O₂^{64, 62, 907}



Molecular weight	86.0892	H bond acceptors	2	Rule of 5 violations	0
Compound type	carboxylic acid	H bond donors	1	ACD/ALogP	0.94
Phase 25°C	solid	Rotatable bonds	1	Predicted density	1.039 g/cm ³
SMILES	<chem>O=C(O)/C=C/C</chem>				
InChIKey	LDHQCZJRKDOVOX-NSCUHMNNSA-N				

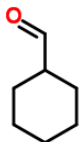
Solubility Data

Solvent	Concentration (M)	Mole Fraction (X)	pph (g/100g)
acetonitrile	3.59	0.22	58.89
benzene	4.45	0.39	69.51
chloroform	7.34	0.60	107.51
DMSO	7.76	0.61	170.26
ethanol	6.15	0.43	138.41
hexane	1.07	0.13	14.97
methanol	7.62	0.47	236.33
THF	8.09	0.66	233.69
toluene	3.52	0.34	49.12
water	0.89	0.02	8.29

cyclohexanecarbaldehyde C₇H₁₂O²¹

Compound Data

Molecular weight	112.17	H bond acceptors	1	Rule of 5 violations	0
Compound type	aldehyde	H bond donors	0	ACD/ALogP	2.02

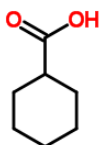


Phase 25°C	liquid	Rotatable bonds	1	Predicted density	0.992 g/cm
SMILES	<chem>C1CCC(CC1)C=O</chem>				
InChIKey	KVFDZFBHBWTVID-UHFFFAOYSA-N				

Solubility Data

Solvent	Concentration (M)	Mole Fraction (X)	pph (g/100g)
methanol	8.29	0.85	1972.34

cyclohexanecarboxylic acid C₇H₁₂O₂²²



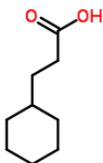
Compound Data

Molecular weight	128.169	H bond acceptors	2	Rule of 5 violations	0
Compound type	carboxylic acid	H bond donors	1	ACD/ALogP	1.88
Phase 25°C	liquid	Rotatable bonds	1	Predicted density	1.079 g/cm ³
SMILES	<chem>C1CCC(CC1)C(=O)O</chem>				
InChIKey	NZNMSOFKMUBTKW-UHFFFAOYSA-N				

Solubility Data

Solvent	Concentration (M)	Mole Fraction (X)	pph (g/100g)
methanol	8.06	0.89	3220.96

cyclohexanepropionic acid C₉H₁₆O₂²²



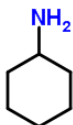
Compound Data

Molecular weight	156.222	H bond acceptors	2	Rule of 5 violations	0
Compound type	carboxylic acid	H bond donors	1	ACD/ALogP	3.09
Phase 25°C	liquid	Rotatable bonds	3	Predicted density	1.006 g/cm ³
SMILES	<chem>C1CCC(CC1)CCC(=O)O</chem>				
InChIKey	HJZLEGIHUQOJBA-UHFFFAOYSA-N				

Solubility Data

Solvent	Concentration (M)	Mole Fraction (X)	pph (g/100g)
methanol	5.84	0.73	1301.33

cyclohexylamine C₆H₁₃N²⁹



Compound Data

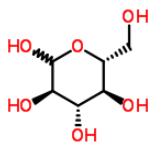
Molecular weight	99.1741	H bond acceptors	1	Rule of 5 violations	0
Compound type	amine	H bond donors	2	ACD/ALogP	1.3
Phase 25°C	liquid	Rotatable bonds	1	Predicted density	0.869 g/cm ³
SMILES	<chem>NC1CCCCC1</chem>				
InChIKey	PAFZNILMFXTMIY-UHFFFAOYSA-N				

Solubility Data

Solvent	Concentration (M)	Mole Fraction (X)	pph (g/100g)
methanol	8.74	0.99	45092.19

D-glucose C₆H₁₂O₆^{1, 207}

Compound Data



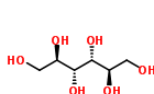
Molecular weight	180.156	H bond acceptors	6	Rule of 5 violations	1
Compound type	non-Ugi related	H bond donors	5	ACD/ALogP	-2.57
Phase 25°C	solid	Rotatable bonds	6	Predicted density	1.732 g/cm ³
SMILES	<chem>O[C@H]1[C@H](O)[C@H](OC(O)[C@@H]1O)CO</chem>				
InChIKey	WQZGKKKJIJFFOK-GASJEMHNSA-N				

Solubility Data

Solvent	Concentration (M)	Mole Fraction (X)	pph (g/100g)
ethanol	0.01	0.00	0.12
methanol	0.04	0.00	0.84
THF	0.02	0.00	0.30

D-mannitol C₆H₁₄O₆^{1, 207}

Compound Data

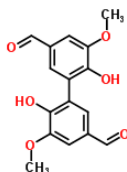


Molecular weight	182.172	H bond acceptors	6	Rule of 5 violations	1
Compound type	non-Ugi related	H bond donors	6	ACD/ALogP	-2.68
Phase 25°C	solid	Rotatable bonds	11	Predicted density	1.596 g/cm ³
SMILES	<chem>O[C@H]([C@H](O)CO)[C@H](O)[C@H](O)CO</chem>				
InChIKey	FBPFZTCFMRRESA-KVTDHHQDSA-N				

Solubility Data

Solvent	Concentration (M)	Mole Fraction (X)	pph (g/100g)
ethanol	0.01	0.00	0.12
methanol	0.01	0.00	0.24
THF	0.02	0.00	0.30

dehydrodivanillin C₁₆H₁₄O₆⁹⁰⁶



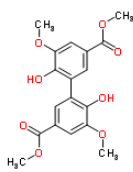
Compound Data

Molecular weight	302.279	H bond acceptors	6	Rule of 5 violations	0
Compound type	non-Ugi related	H bond donors	2	ACD/ALogP	2.7
Phase 25°C	solid	Rotatable bonds	7	Predicted density	1.356 g/cm ³
SMILES	<chem>O=Cc2cc(c1cc(cc(OC)c1O)C=O)c(O)c(OC)c2</chem>				
InChIKey	NSTQUZVZBUTVPY-UHFFFAOYSA-N				

Solubility Data

Solvent	Concentration (M)	Mole Fraction (X)	pph (g/100g)
1-propanol	0.00	0.00	0.00
1,2-dichloroethane	0.00	0.00	0.00
butanone	0.00	0.00	0.00
toluene	0.00	0.00	0.00

di(methyl vanillate) C₁₈H₁₈O₈⁹⁰⁶



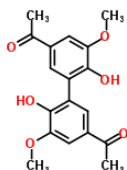
Compound Data

Molecular weight	362.331	H bond acceptors	8	Rule of 5 violations	0
Compound type	non-Ugi related	H bond donors	2	ACD/ALogP	2.28
Phase 25°C	solid	Rotatable bonds	9	Predicted density	1.315 g/cm ³
SMILES	<chem>O=C(OC)c2cc(c1cc(cc(OC)c1O)C(=O)OC)c(O)c(OC)c2</chem>				
InChIKey	DBUKZZKLTXIQM-UHFFFAOYSA-N				

Solubility Data

Solvent	Concentration (M)	Mole Fraction (X)	pph (g/100g)
1-propanol	0.00	0.00	0.00
1,2-dichloroethane	0.01	0.00	0.31
butanone	0.00	0.00	0.00
toluene	0.00	0.00	0.00

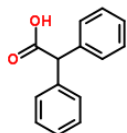
diapocynin C₁₈H₁₈O₆⁹⁰⁶



Compound Data			
Molecular weight	330.332	H bond acceptors	6
Compound type	non-Ugi related	Rule of 5 violations	0
Phase 25°C	solid	H bond donors	2
SMILES	<chem>O=C(c2cc(c1cc(cc(OC)c1O)C(=O)C)c(O)c(OC)c2)C</chem>		
InChIKey	HLNDPICGHQGSU-UHFFFAOYSA-N		
	Rotatable bonds	ACD/ALogP	2.84
	7	Predicted density	1.257 g/cm ³

Solubility Data			
Solvent	Concentration (M)	Mole Fraction (X)	pph (g/100g)
1-propanol	0.00	0.00	0.00
1,2-dichloroethane	0.00	0.00	0.00
butanone	0.00	0.00	0.00
toluene	0.00	0.00	0.00

diphenylacetic acid C₁₄H₁₂O₂^{81, 77, 907}



Compound Data			
Molecular weight	212.244	H bond acceptors	2
Compound type	carboxylic acid	Rule of 5 violations	0
Phase 25°C	solid	H bond donors	1
SMILES	<chem>O=C(O)C(c1ccccc1)c2ccccc2</chem>		
InChIKey	PYHXGXCGESYPCW-UHFFFAOYSA-N		
	Rotatable bonds	ACD/ALogP	2.79
	3	Predicted density	1.174 g/cm ³

Solubility Data			
Solvent	Concentration (M)	Mole Fraction (X)	pph (g/100g)
acetonitrile	0.46	0.03	14.26
DMSO	2.56	0.25	92.04
ethanol	1.15	0.08	39.51
methanol	1.27	0.07	46.47
THF	2.91	0.33	144.17
toluene	0.17	0.02	4.27
water	0.00	0.00	0.00

formic acid CH₂O₂²²

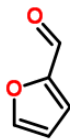


Compound Data			
Molecular weight	46.0254	H bond acceptors	2
Compound type	carboxylic acid	Rule of 5 violations	0
Phase 25°C	liquid	H bond donors	1
SMILES	<chem>O=CO</chem>		
InChIKey	BDAGIHXWWSANSR-UHFFFAOYSA-N		
	Rotatable bonds	ACD/ALogP	-0.47
	0	Predicted density	1.154 g/cm ³

Solubility Data			
Solvent	Concentration (M)	Mole Fraction (X)	pph (g/100g)
methanol	26.50	□	□

□ Solute is very soluble/miscible, conversion fail.

furfuraldehyde C₅H₄O₂²⁰



Compound Data

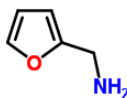
Molecular weight	96.0841	H bond acceptors	2	Rule of 5 violations	0
Compound type	aldehyde	H bond donors	0	ACD/ALogP	0.43
Phase 25°C	liquid	Rotatable bonds	1	Predicted density	1.145 g/cm ³
SMILES	<chem>O=Cc1ccco1</chem>				
InChIKey	HYBBIBNJHNGZAN-UHFFFAOYSA-N				

Solubility Data

Solvent	Concentration (M)	Mole Fraction (X)	pph (g/100g)
methanol	12.02	□	□

□ Solute is very soluble/miscible, conversion fail.

furfurylamine C₅H₇NO²⁶



Compound Data

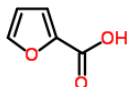
Molecular weight	97.1152	H bond acceptors	2	Rule of 5 violations	0
Compound type	amine	H bond donors	2	ACD/ALogP	-0.43
Phase 25°C	liquid	Rotatable bonds	2	Predicted density	1.053 g/cm ³
SMILES	<chem>NCc1ccco1</chem>				
InChIKey	DDRPCXLAQZKBJP-UHFFFAOYSA-N				

Solubility Data

Solvent	Concentration (M)	Mole Fraction (X)	pph (g/100g)
methanol	11.32	□	□

□ Solute is very soluble/miscible, conversion fail.

furoic acid C₅H₄O₃^{104, 911}



Compound Data

Molecular weight	112.084	H bond acceptors	3	Rule of 5 violations	0
Compound type	carboxylic acid	H bond donors	1	ACD/ALogP	0.98
Phase 25°C	solid	Rotatable bonds	1	Predicted density	1.322 g/cm ³
SMILES	<chem>OC(=O)c1ccco1</chem>				
InChIKey	SMNDYUVBFMFKNZ-UHFFFAOYSA-N				

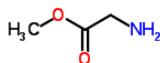
Solubility Data

Solvent	Concentration (M)	Mole Fraction (X)	pph (g/100g)
acetonitrile	1.10	0.06	18.14
DMSO	6.64	0.52	154.95
methanol	4.12	0.21	94.36
THF	4.07	0.33	77.05
toluene	0.06	0.01	0.78
water	0.32	0.03	4.23

glycine methyl ester C₃H₇NO₂²⁰⁷

Compound Data

Molecular weight	89.0932	H bond acceptors	3	Rule of 5 violations	0
Compound type	amine	H bond donors	2	ACD/ALogP	-1.37
Phase 25°C	solid	Rotatable bonds	3	Predicted density	1.045 g/cm ³



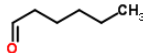
SMILES O=C(OC)CN
InChIKey KQSSATDQUYCRGS-UHFFFAOYSA-N

Solubility Data

Solvent	Concentration (M)	Mole Fraction (X)	pph (g/100g)
ethanol	0.19	0.01	2.21
methanol	1.32	0.06	17.60
THF	0.04	0.00	0.40

hexanaldehyde $C_6H_{12}O^{21}$

Compound Data

	Molecular weight 100.159	H bond acceptors 1	Rule of 5 violations 0
Compound type aldehyde	H bond donors 0	ACD/ALogP 2.37	
Phase 25°C liquid	Rotatable bonds 4	Predicted density 0.801 g/cm ³	
SMILES <chem>CCCCCC=O</chem>			
InChIKey <chem>JARKCYVAAOWBJS-UHFFFAOYSA-N</chem>			

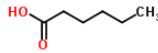
Solubility Data

Solvent	Concentration (M)	Mole Fraction (X)	pph (g/100g)
methanol	8.33	□	□

□ Solute is very soluble/miscible, conversion fail.

hexanoic acid $C_6H_{12}O_2^{22}$

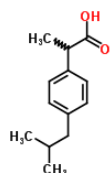
Compound Data

	Molecular weight 116.158	H bond acceptors 2	Rule of 5 violations 0
Compound type carboxylic acid	H bond donors 1	ACD/ALogP 1.88	
Phase 25°C liquid	Rotatable bonds 4	Predicted density 0.95 g/cm ³	
SMILES <chem>CCCCCC(=O)O</chem>			
InChIKey <chem>FUZZWVXGSFPDMH-UHFFFAOYSA-N</chem>			

Solubility Data

Solvent	Concentration (M)	Mole Fraction (X)	pph (g/100g)
methanol	7.98	0.93	5071.51

ibuprofen $C_{13}H_{18}O_2^{905, 907}$



Compound Data

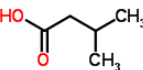
Molecular weight 206.281	H bond acceptors 2	Rule of 5 violations 0
Compound type carboxylic acid	H bond donors 1	ACD/ALogP 3.5
Phase 25°C solid	Rotatable bonds 4	Predicted density 1.029 g/cm ³
SMILES <chem>O=C(O)C(c1ccc(cc1)CC(C)C)C</chem>		
InChIKey <chem>HEFNNWSXXWATRW-UHFFFAOYSA-N</chem>		

Solubility Data

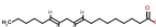
Solvent	Concentration (M)	Mole Fraction (X)	pph (g/100g)
1-decanol	1.12	0.22	35.98
1-octanol	1.20	0.20	39.60

1-pentanol	1.46	0.18	52.50
1-propanol	1.52	0.14	56.72
2-butanol	1.78	0.20	71.27
2-methyl-1-propanol	1.76	0.20	70.04
2-propanol	2.22	0.23	104.32
ethanol	1.18	0.08	40.88
methanol	1.16	0.06	41.41
water	0.00	0.00	0.00

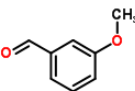
isovaleric acid C₅H₁₀O₂²²

	Compound Data				
	Molecular weight	102.132	H bond acceptors	2 Rule of 5 violations	0
	Compound type	carboxylic acid	H bond donors	1 ACD/ALogP	1.26
	Phase 25°C	liquid	Rotatable bonds	2 Predicted density	0.962 g/cm³
	SMILES	CC(C)CC(=O)O			
	InChIKey	GWYFCOCPABKNJV-UHFFFAOYSA-N			
Solubility Data					
Solvent	Concentration (M)	Mole Fraction (X)	pph (g/100g)		
methanol	9.06	0.91	3222.50		

linoleic acid C₁₈H₃₂O₂²²

Compound Data						
	Molecular weight	280.445	H bond acceptors	2	Rule of 5 violations	1
	Compound type	carboxylic acid	H bond donors	1	ACD/ALogP	7.06
	Phase 25°C	liquid	Rotatable bonds	14	Predicted density	0.911 g/cm ³
	SMILES	CCCCC=CCC=CCCCCCCC(=O)O				
	InChIKey	OYHQOLUKZRVURQ-AVQMFATSA-N				
Solubility Data						
Solvent	Concentration (M)	Mole Fraction (X)	pph (g/100g)			
methanol	3.22	0.94	13712.82			

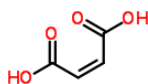
m-anisaldehyde C₈H₈O₂²¹

Compound Data				
	Molecular weight	136.148	H bond acceptors	2 Rule of 5 violations 0
	Compound type	aldehyde	H bond donors	0 ACD/ALogP 1.62
	Phase 25°C	liquid	Rotatable bonds	2 Predicted density 1.088 g/cm³
	SMILES	COc1cc(C=O)ccc1		
	InChIKey	WMPDAIZRQDCGFH-UHFFFAOYSA-N		
Solubility Data				
Solvent	Concentration (M)	Mole Fraction (X)	pph (g/100g)	
methanol	8.20	□	□	

□ Solute is very soluble/miscible, conversion fail.

maleic acid C₄H₄O₄^{39, 40}

Compound Data			
Molecular weight	116.072	H bond acceptors 4 Rule of 5 violations 0	
Compound type	carboxylic acid	H bond donors 2 ACD/ALogP 0.21	

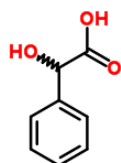


Phase 25°C	solid	Rotatable bonds	2	Predicted density	1.499 g/cm ³
SMILES	<chem>C(=CC(=O)O)C(=O)O</chem>				
InChIKey	VZCYOOQTPOCHFL-OWOJBTEDSA-N				

Solubility Data

Solvent	Concentration (M)	Mole Fraction (X)	pph (g/100g)
ethanol	3.41	0.21	68.95
methanol	3.82	0.19	83.62

mandelic acid C₈H₈O₃^{72, 71}

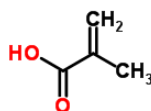


Compound Data					
Molecular weight	152.147	H bond acceptors	3	Rule of 5 violations	0
Compound type	carboxylic acid	H bond donors	2	ACD/ALogP	0.66
Phase 25°C	solid	Rotatable bonds	3	Predicted density	1.321 g/cm ³
SMILES	<chem>O=C(O)C(O)c1ccccc1</chem>				
InChIKey	IWYDHOAUDWTVEP-UHFFFAOYSA-N				

Solubility Data

Solvent	Concentration (M)	Mole Fraction (X)	pph (g/100g)
1-hexanol	0.00	0.00	0.00
chloroform	0.12	0.01	1.23
diethyl ether	0.77	0.08	17.51
methanol	3.54	0.20	120.77
toluene	0.00	0.00	0.00

methacrylic acid C₄H₆O₂²²

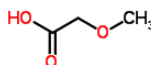


Compound Data					
Molecular weight	86.0892	H bond acceptors	2	Rule of 5 violations	0
Compound type	carboxylic acid	H bond donors	1	ACD/ALogP	0.63
Phase 25°C	liquid	Rotatable bonds	1	Predicted density	1.023 g/cm ³
SMILES	<chem>CC(=C)C(=O)O</chem>				
InChIKey	CERQOIWHTDAKMF-UHFFFAOYSA-N				

Solubility Data

Solvent	Concentration (M)	Mole Fraction (X)	pph (g/100g)
methanol	11.79	0.98	17218.73

methoxyacetic acid C₃H₆O₃²²



Compound Data					
Molecular weight	90.0779	H bond acceptors	3	Rule of 5 violations	0
Compound type	carboxylic acid	H bond donors	1	ACD/ALogP	-0.49
Phase 25°C	liquid	Rotatable bonds	2	Predicted density	1.139 g/cm ³
SMILES	<chem>COCC(=O)O</chem>				
InChIKey	RMIODHQZRUFFFF-UHFFFAOYSA-N				

Solubility Data

Solvent	Concentration (M)	Mole Fraction (X)	pph (g/100g)
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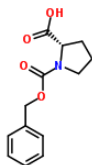
methanol

13.03

□

□

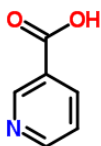
□ Solute is very soluble/miscible, conversion fail.

N-Cbz-L-p roline C₁₃H₁₅NO₄¹³⁴**Compound Data**

Molecular weight	249.262	H bond acceptors	5	Rule of 5 violations	0
Compound type	carboxylic acid	H bond donors	1	ACD/ALogP	1.21
Phase 25°C	solid	Rotatable bonds	4	Predicted density	1.309 g/cm ³
SMILES	O=C(O)[C@H]2N(C(=O)OCc1ccccc1)CCC2				
InChIKey	JXGVXCZADZNAMJ-NSHDSACASA-N				

Solubility Data

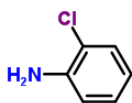
Solvent	Concentration (M)	Mole Fraction (X)	pph (g/100g)
methanol	4.26	0.49	746.90

nicotinic acid C₆H₅NO₂^{100, 137, 907}**Compound Data**

Molecular weight	123.109	H bond acceptors	3	Rule of 5 violations	0
Compound type	carboxylic acid	H bond donors	1	ACD/ALogP	0.29
Phase 25°C	solid	Rotatable bonds	1	Predicted density	1.293 g/cm ³
SMILES	O=C(O)c1ccncc1				
InChIKey	PVNIIMVLHYAWGP-UHFFFAOYSA-N				

Solubility Data

Solvent	Concentration (M)	Mole Fraction (X)	pph (g/100g)
acetonitrile	0.00	0.00	0.00
benzene	0.00	0.00	0.00
DMSO	0.57	0.04	6.71
ethanol	0.09	0.01	1.43
methanol	0.06	0.00	1.03
THF	0.06	0.00	0.75
toluene	0.00	0.00	0.00
water	0.37	0.01	4.73

o-chloroaniline C₆H₆ClN²⁹**Compound Data**

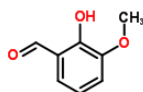
Molecular weight	127.572	H bond acceptors	1	Rule of 5 violations	0
Compound type	amine	H bond donors	2	ACD/ALogP	1.93
Phase 25°C	liquid	Rotatable bonds	1	Predicted density	1.23 g/cm ³
SMILES	Nc1ccccc1Cl				
InChIKey	AKCRQHGGQJBRMN-UHFFFAOYSA-N				

Solubility Data

Solvent	Concentration (M)	Mole Fraction (X)	pph (g/100g)
methanol	9.51	0.97	11802.88

o-vanillin C₈H₈O₃^{208, 205}**Compound Data**

Molecular weight	152.147	H bond acceptors	3	Rule of 5 violations	0
Compound type	aldehyde	H bond donors	1	ACD/ALogP	1.31

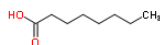


Phase 25°C	solid	Rotatable bonds	3	Predicted density	1.231 g/cm ³
SMILES	<chem>Oc1c(cccc1OC)C=O</chem>				
InChIKey	JJVNINGBHBWJH-UHFFFAOYSA-N				

Solubility Data

Solvent	Concentration (M)	Mole Fraction (X)	pph (g/100g)
acetonitrile	2.56	0.17	76.28
ethanol	3.04	0.22	94.99
methanol	2.27	0.12	63.75
THF	5.37	0.56	268.76
toluene	3.82	0.43	126.41

octanoic acid C₈H₁₆O₂²²



Molecular weight	144.211	H bond acceptors	2	Rule of 5 violations	0
Compound type	carboxylic acid	H bond donors	1	ACD/ALogP	2.92
Phase 25°C	liquid	Rotatable bonds	6	Predicted density	0.929 g/cm ³
SMILES	<chem>CCCCCCC(=O)O</chem>				
InChIKey	WWZKQHOCKIZLMA-UHFFFAOYSA-N				

Solubility Data

Solvent	Concentration (M)	Mole Fraction (X)	pph (g/100g)
methanol	6.31	0.93	5899.86

octylamine C₈H₁₉N²⁹

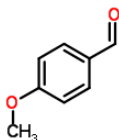


Molecular weight	129.243	H bond acceptors	1	Rule of 5 violations	0
Compound type	amine	H bond donors	2	ACD/ALogP	3.24
Phase 25°C	liquid	Rotatable bonds	7	Predicted density	0.786 g/cm ³
SMILES	<chem>NCCCCCCC</chem>				
InChIKey	IOQPZZOEVPZRBK-UHFFFAOYSA-N				

Solubility Data

Solvent	Concentration (M)	Mole Fraction (X)	pph (g/100g)
methanol	6.05	0.98	20005.33

p-anisaldehyde C₈H₈O₂²¹



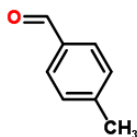
Molecular weight	136.148	H bond acceptors	2	Rule of 5 violations	0
Compound type	aldehyde	H bond donors	0	ACD/ALogP	1.64
Phase 25°C	liquid	Rotatable bonds	2	Predicted density	1.088 g/cm ³
SMILES	<chem>COc1ccc(C=O)cc1</chem>				
InChIKey	ZRSNZINYAWTAHE-UHFFFAOYSA-N				

Solubility Data

Solvent	Concentration (M)	Mole Fraction (X)	pph (g/100g)
methanol	8.22	□	□

□ Solute is very soluble/miscible, conversion fail.

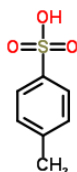
p-tolualdehyde C₈H₈O²¹



Compound Data					
Molecular weight	120.148	H bond acceptors	1	Rule of 5 violations	0
Compound type	aldehyde	H bond donors	0	ACD/ALogP	2.01
Phase 25°C	liquid	Rotatable bonds	1	Predicted density	1.023 g/cm ³
SMILES	O=Cc1ccc(C)cc1				
InChIKey	FXLOVSHXALFLKQ-UHFFFAOYSA-N				

Solubility Data			
Solvent	Concentration (M)	Mole Fraction (X)	pph (g/100g)
methanol	8.47	0.99	25859.25

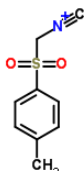
p-toluenesulfonic acid C₇H₈O₃S^{107, 136}



Compound Data					
Molecular weight	172.202	H bond acceptors	3	Rule of 5 violations	0
Compound type	non-Ugi related	H bond donors	1	ACD/ALogP	-0.88
Phase 25°C	solid	Rotatable bonds	1	Predicted density	1.34 g/cm ³
SMILES	O=S(=O)(O)c1ccc(cc1)C				
InChIKey	JOXIMZWYDAKGHI-UHFFFAOYSA-N				

Solubility Data			
Solvent	Concentration (M)	Mole Fraction (X)	pph (g/100g)
acetonitrile	0.11	0.01	2.69
ethanol	4.69	0.41	260.62
toluene	0.00	0.00	0.00

p-toluenesulfonylmethyl isocyanide C₉H₉NO₂S²⁰⁸



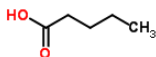
Compound Data					
Molecular weight	195.238	H bond acceptors	3	Rule of 5 violations	0
Compound type	isonitrile	H bond donors	0	ACD/ALogP	1.38
Phase 25°C	solid	Rotatable bonds	2	Predicted density	‡
SMILES	O=S(=O)(c1ccc(cc1)C)C[N+]#[C-]				
InChIKey	CFOAUYCPAUGDFF-UHFFFAOYSA-N				

Solubility Data			
Solvent	Concentration (M)	Mole Fraction (X)	pph (g/100g)
acetonitrile	1.88	‡	‡
chloroform	0.21	‡	‡
ethanol	0.18	‡	‡
THF	1.86	‡	‡
toluene	0.14	‡	‡

‡ Solute density prediction fail.

pentanoic acid C₅H₁₀O₂²²

Compound Data					
Molecular weight	102.132	H bond acceptors	2	Rule of 5 violations	0
Compound type	carboxylic acid	H bond donors	1	ACD/ALogP	1.34
Phase 25°C	liquid	Rotatable bonds	3	Predicted density	0.966 g/cm ³

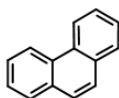


SMILES CCCCC(=O)O
InChIKey NQPDZGIKBAWPEJ-UHFFFAOYSA-N

Solubility Data

Solvent	Concentration (M)	Mole Fraction (X)	pph (g/100g)
methanol	9.19	0.93	4393.39

phenanthrene C₁₄H₁₀⁹⁰²



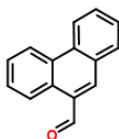
Compound Data

Molecular weight 178.229 **H bond acceptors** 0 **Rule of 5 violations** 0
Compound type non-Ugi related **H bond donors** 0 **ACD/ALogP** 4.55
Phase 25°C solid **Rotatable bonds** 0 **Predicted density** 1.13 g/cm³
SMILES c3cc2ccc1ccccc1c2cc3
InChIKey YNPNZTXNASCQKK-UHFFFAOYSA-N

Solubility Data

Solvent	Concentration (M)	Mole Fraction (X)	pph (g/100g)
benzene	2.02	0.21	60.52
carbon disulfide	3.05	0.26	83.20
carbon tetrachloride	1.73	0.18	24.99
diethyl ether	1.36	0.15	42.04
ethanol	0.21	0.01	4.96
hexane	0.32	0.04	8.90

phenanthrene-9-carboxaldehyde C₁₅H₁₀O^{30, 60, 136, 4, 242, 51, 24}



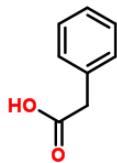
Compound Data

Molecular weight 206.239 **H bond acceptors** 1 **Rule of 5 violations** 0
Compound type aldehyde **H bond donors** 0 **ACD/ALogP** 4.28
Phase 25°C solid **Rotatable bonds** 1 **Predicted density** 1.217 g/cm³
SMILES O=Cc2cc3c(c1c2ccccc1)cccc3
InChIKey QECIGCMPORCORE-UHFFFAOYSA-N

Solubility Data

Solvent	Concentration (M)	Mole Fraction (X)	pph (g/100g)
1,1,2-trichlorotrifluoroethane	0.02	0.00	0.25
2-propanol	0.07	0.01	1.85
acetonitrile	0.16	0.01	4.39
benzene	0.66	0.06	17.56
chloroform	0.04	0.00	0.55
cyclohexane	0.07	0.01	1.85
cyclopentane	0.03	0.00	0.79
dichloromethane	0.00	0.00	0.00
diethyl ether	0.10	0.01	2.86
DMF	1.25	0.12	37.60
DMSO	0.77	0.06	16.62
ethanol	0.10	0.01	2.69
hexane	0.07	0.01	2.16
methanol	0.11	0.00	2.93
THF	2.32	0.23	87.22
toluene	0.14	0.01	3.40

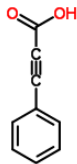
phenylacetic acid C₈H₈O₂^{86, 123, 907}



Compound Data			
Molecular weight	136.148	H bond acceptors	2 Rule of 5 violations 0
Compound type	carboxylic acid	H bond donors	1 ACD/ALogP 1.72
Phase 25°C	solid	Rotatable bonds	2 Predicted density 1.164 g/cm ³
SMILES	O=C(O)Cc1ccccc1		
InChIKey	WLJVXDMOQOGPHL-UHFFFAOYSA-N		

Solubility Data			
Solvent	Concentration (M)	Mole Fraction (X)	pph (g/100g)
acetonitrile	3.87	0.28	128.87
benzene	3.35	0.33	85.91
DMF	3.76	0.36	105.03
DMSO	6.35	0.64	305.77
THF	5.62	0.57	247.02
toluene	1.94	0.21	39.23
water	0.13	0.00	1.80

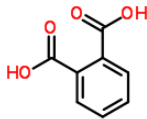
phenylpropynoic acid C₉H₆O₂^{98, 82, 85}



Compound Data			
Molecular weight	146.143	H bond acceptors	2 Rule of 5 violations 0
Compound type	carboxylic acid	H bond donors	1 ACD/ALogP 1.7
Phase 25°C	solid	Rotatable bonds	1 Predicted density 1.24 g/cm ³
SMILES	O=C(C#Cc1ccccc1)O		
InChIKey	XNERWVPQCYSMLC-UHFFFAOYSA-N		

Solubility Data			
Solvent	Concentration (M)	Mole Fraction (X)	pph (g/100g)
acetonitrile	1.38	0.08	32.24
DMSO	3.33	0.28	72.89
methanol	2.89	0.16	85.06
THF	4.34	0.42	143.85

phthalic acid C₈H₆O₄^{138, 47}

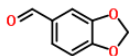


Compound Data			
Molecular weight	166.131	H bond acceptors	4 Rule of 5 violations 0
Compound type	carboxylic acid	H bond donors	2 ACD/ALogP 1.22
Phase 25°C	solid	Rotatable bonds	2 Predicted density 1.451 g/cm ³
SMILES	O=C(O)c1ccccc1C(=O)O		
InChIKey	XNGIFLGASWRNHJ-UHFFFAOYSA-N		

Solubility Data			
Solvent	Concentration (M)	Mole Fraction (X)	pph (g/100g)
chloroform	0.51	0.04	6.00
methanol	0.43	0.02	9.98

piperal C₈H₆O₃^{71, 30, 907}

Compound Data			
Molecular weight	150.131	H bond acceptors	3 Rule of 5 violations 0
Compound type	aldehyde	H bond donors	0 ACD/ALogP 0.79

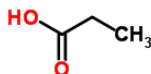


Phase 25°C	solid	Rotatable bonds	1	Predicted density	1.337 g/cm ³
SMILES	<chem>O=Cc1ccc2OCOc2c1</chem>				
InChIKey	SATCULPHIDQDRE-UHFFFAOYSA-N				

Solubility Data

Solvent	Concentration (M)	Mole Fraction (X)	pph (g/100g)
acetonitrile	7.11	0.66	708.73
chloroform	7.95	0.86	741.57
dichloromethane	7.59	0.78	616.11
diethyl ether	6.38	0.69	460.15
DMSO	6.05	0.57	257.75
ethanol	4.99	0.40	218.45
hexane	0.15	0.02	3.39
methanol	7.29	0.63	798.18
THF	7.44	0.78	750.82
toluene	6.40	0.71	392.09
water	0.02	0.00	0.30

propanoic acid C₃H₆O₂²²



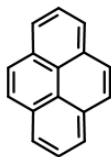
Compound Data

Molecular weight	74.0785	H bond acceptors	2	Rule of 5 violations	0
Compound type	carboxylic acid	H bond donors	1	ACD/ALogP	0.31
Phase 25°C	liquid	Rotatable bonds	1	Predicted density	1.019 g/cm ³
SMILES	<chem>CCC(=O)O</chem>				
InChIKey	XBDQKXXYIPTUBI-UHFFFAOYSA-N				

Solubility Data

Solvent	Concentration (M)	Mole Fraction (X)	pph (g/100g)
methanol	13.41	0.96	5249.72

pyrene C₁₆H₁₀^{108, 109}



Compound Data

Molecular weight	202.251	H bond acceptors	0	Rule of 5 violations	1
Compound type	non-Ugi related	H bond donors	0	ACD/ALogP	5.19
Phase 25°C	solid	Rotatable bonds	0	Predicted density	1.248 g/cm ³
SMILES	<chem>c3ccc2ccc1cccc4c1c2c3cc4</chem>				
InChIKey	BBEAQIROQSPTKN-UHFFFAOYSA-N				

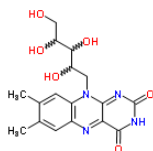
Solubility Data

Solvent	Concentration (M)	Mole Fraction (X)	pph (g/100g)
acetonitrile	0.10	0.01	2.75

riboflavin C₁₇H₂₀N₄O₆⁴⁶

Compound Data

Molecular weight	376.364	H bond acceptors	10	Rule of 5 violations	2
Compound type	non-Ugi related	H bond donors	5	ACD/ALogP	-2.02
Phase 25°C	solid	Rotatable bonds	9	Predicted density	1.65 g/cm ³
SMILES	<chem>O=C2/N=C1/N(c3cc(cc3/N=C1C(=O)N2)C)CC(O)C(O)C(O)CO</chem>				

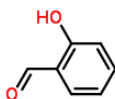


InChIKey AUNGANRZJHBGPY-UHFFFAOYSA-N

Solubility Data

Solvent	Concentration (M)	Mole Fraction (X)	pph (g/100g)
methanol	0.00	0.00	0.00

salicylaldehyde C₇H₆O₂²¹



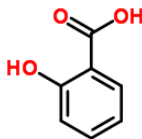
Molecular weight	122.121	H bond acceptors	2	Rule of 5 violations	0
Compound type	aldehyde	H bond donors	1	ACD/ALogP	1.61
Phase 25°C	liquid	Rotatable bonds	2	Predicted density	1.226 g/cm ³
SMILES	c1cccc(C=O)c1O				
InChIKey	SMQUZDBALVYZAC-UHFFFAOYSA-N				

Solubility Data

Solvent	Concentration (M)	Mole Fraction (X)	pph (g/100g)
methanol	10.04	□	□

□ Solute is very soluble/miscible, conversion fail.

salicylic acid C₇H₆O₃^{34, 902, 901, 138, 52, 907}

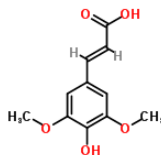


Molecular weight	138.121	H bond acceptors	3	Rule of 5 violations	0
Compound type	carboxylic acid	H bond donors	2	ACD/ALogP	2.06
Phase 25°C	solid	Rotatable bonds	2	Predicted density	1.375 g/cm ³
SMILES	O=C(O)c1ccccc1O				
InChIKey	YGSDEFSMJLZEOE-UHFFFAOYSA-N				

Solubility Data

Solvent	Concentration (M)	Mole Fraction (X)	pph (g/100g)
chloroform	0.19	0.01	1.74
dichloromethane	0.15	0.01	1.68
ethanol	2.34	0.15	54.17
methanol	2.65	0.13	66.24
toluene	0.11	0.01	1.76
water	0.01	0.00	0.14

sinapic acid C₁₁H₁₂O₅^{25, 2}



Molecular weight	224.21	H bond acceptors	5	Rule of 5 violations	0
Compound type	carboxylic acid	H bond donors	2	ACD/ALogP	1.29
Phase 25°C	solid	Rotatable bonds	5	Predicted density	1.307 g/cm ³
SMILES	O=C(O)\C=C\c1cc(OC)c(O)c(OC)c1				
InChIKey	PCMORTLOPMLFEB-ONEGZZNKSA-N				

Solubility Data

Solvent	Concentration	Mole Fraction (X)	pph (g/100g)
		48	

	(M)		
ethanol	0.79	0.05	26.27
methanol	1.04	0.05	37.69
THF	0.45	0.04	11.95

sodium chloride $\text{CINa}^{1, 207, 900}$

Compound Data

	Molecular weight	58.4428	H bond acceptors	0	Rule of 5 violations	0
	Compound type	non-Ugi related	H bond donors	0	ACD/ALogP	†
	Phase 25°C	solid	Rotatable bonds	0	Predicted density	‡
	SMILES	<chem>[Cl][Na]</chem>				
InChIKey		FAPWRFPIFSIZLT-UHFFFAOYSA-M				

Solubility Data

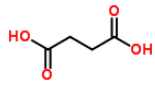
Solvent	Concentration (M)	Mole Fraction (X)	pph (g/100g)
ethanol	0.00	0.00	0.00
methanol	0.21	‡	‡
THF	0.04	‡	‡

† ACD/ALogP prediction fail.

‡ Solute density prediction fail.

succinic acid $\text{C}_4\text{H}_6\text{O}_4^{45, 44, 42}$

Compound Data

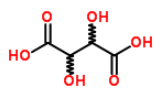
	Molecular weight	118.088	H bond acceptors	4	Rule of 5 violations	0
	Compound type	carboxylic acid	H bond donors	2	ACD/ALogP	-0.59
	Phase 25°C	solid	Rotatable bonds	3	Predicted density	1.408 g/cm ³
	SMILES	<chem>OC(=O)CCC(=O)O</chem>				
	InChIKey	KDYFGRWQOYBRFD-UHFFFAOYSA-N				

Solubility Data

Solvent	Concentration (M)	Mole Fraction (X)	pph (g/100g)
2-propanol	0.34	0.03	5.22
ethanol	0.57	0.03	9.06

tartaric acid $\text{C}_4\text{H}_6\text{O}_6^{38}$

Compound Data

	Molecular weight	150.087	H bond acceptors	6	Rule of 5 violations	0
	Compound type	carboxylic acid	H bond donors	4	ACD/ALogP	-1.43
	Phase 25°C	solid	Rotatable bonds	5	Predicted density	1.886 g/cm ³
	SMILES	<chem>C(C(=O)O)C(=O)O</chem>				
	InChIKey	FEWJPZIEWOKRBE-UHFFFAOYSA-N				

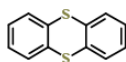
Solubility Data

Solvent	Concentration (M)	Mole Fraction (X)	pph (g/100g)
acetone	0.79	0.06	16.39

thianthrene $\text{C}_{12}\text{H}_8\text{S}_2^{905}$

Compound Data

Molecular weight	216.322	H bond acceptors	0	Rule of 5 violations	0
Compound type	non-Ugi related	H bond donors	0	ACD/ALogP	4.57



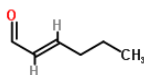
Phase 25°C	solid	Rotatable bonds	0	Predicted density	1.31 g/cm ³
SMILES	S1c3c(Sc2c1cccc2)cccc3				
InChIKey	GVIJJXMTUZIOD-UHFFFAOYSA-N				

Solubility Data

Solvent	Concentration (M)	Mole Fraction (X)	pph (g/100g)
1-decanol	0.04	0.01	1.05
1,4-dioxane	0.27	0.02	6.14
acetonitrile	0.02	0.00	0.58
decane	0.03	0.01	0.89
diethyl ether	0.08	0.01	2.39
diisopropyl ether	0.05	0.01	1.44
ethylene glycol	0.02	0.00	0.40
hexadecane	0.03	0.01	0.84
nonane	0.03	0.01	0.90
undecane	0.03	0.01	0.88

trans-2-hexen-1-al C₆H₁₀O²²

Compound Data



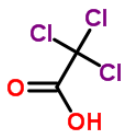
Molecular weight	98.143	H bond acceptors	1	Rule of 5 violations	0
Compound type	aldehyde	H bond donors	0	ACD/ALogP	1.58
Phase 25°C	liquid	Rotatable bonds	3	Predicted density	0.828 g/cm ³
SMILES	CCCC=CC=O				
InChIKey	MBDOYVRWFFCFHM-SNAWJCMRSA-N				

Solubility Data

Solvent	Concentration (M)	Mole Fraction (X)	pph (g/100g)
methanol	8.62	□	□

□ Solute is very soluble/miscible, conversion fail.

trichloroacetic acid C₂HCl₃O₂²²



Compound Data

Molecular weight	163.387	H bond acceptors	2	Rule of 5 violations	0
Compound type	carboxylic acid	H bond donors	1	ACD/ALogP	1.67
Phase 25°C	liquid	Rotatable bonds	0	Predicted density	1.807 g/cm ³
SMILES	C(=O)(C(Cl)(Cl)Cl)O				
InChIKey	YNJBWRMUSHSURL-UHFFFAOYSA-N				

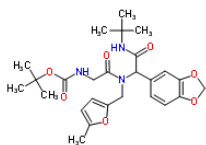
Solubility Data

Solvent	Concentration (M)	Mole Fraction (X)	pph (g/100g)
methanol	9.91	0.80	2068.61

UCExp216-3A C₂₆H₃₅N₃O₇¹¹³

Compound Data

Molecular weight	501.572	H bond acceptors	10	Rule of 5 violations	2
Compound type	Ugi Product	H bond donors	2	ACD/ALogP	4.06
Phase 25°C	solid	Rotatable bonds	10	Predicted density	1.209 g/cm ³

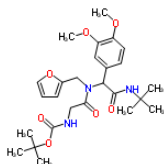


SMILES CC(C)(C)NC(=O)C(c1ccc2OCOc2c1)N(Cc3ccc(C)oc3)C(=O)CNC(=O)OC(C)(C)C
InChIKey MTSJLRXXXJHLDI-UHFFFAOYSA-N

Solubility Data

Solvent	Concentration (M)	Mole Fraction (X)	pph (g/100g)
acetonitrile	0.04	0.00	2.73
DMSO	0.28	0.02	14.46
ethanol	0.03	0.00	1.95
methanol	0.06	0.00	4.10
toluene	0.01	0.00	0.58

Ugi product 104C (UC) $C_{26}H_{37}N_3O_7$ ⁶⁵



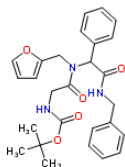
Compound Data

Molecular weight	503.588	H bond acceptors	10	Rule of 5 violations	2
Compound type	Ugi Product	H bond donors	2	ACD/ALogP	3.48
Phase 25°C	solid	Rotatable bonds	12	Predicted density	1.156 g/cm ³
SMILES	<chem>O=C(CNC(=O)OC(C)(C)C)N(Cc1cccc1)C(c2ccc(OC)c(OC)c2)C(=O)NC(C)(C)C</chem>				
InChIKey	<chem>RXLIYJRDQONCRV-UHFFFAOYSA-N</chem>				

Solubility Data

Solvent	Concentration (M)	Mole Fraction (X)	pph (g/100g)
methanol	0.29	0.01	22.20

Ugi product 108C (UC) $C_{27}H_{31}N_3O_5$ ⁶⁵



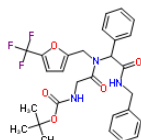
Compound Data

Molecular weight	477.552	H bond acceptors	8	Rule of 5 violations	0
Compound type	Ugi Product	H bond donors	2	ACD/ALogP	4.43
Phase 25°C	solid	Rotatable bonds	11	Predicted density	1.198 g/cm ³
SMILES	<chem>O=C(CNC(=O)OC(C)(C)C)N(Cc1cccc1)C(c2ccccc2)C(=O)NCc3ccccc3</chem>				
InChIKey	<chem>COBIEQVPXUIPRH-UHFFFAOYSA-N</chem>				

Solubility Data

Solvent	Concentration (M)	Mole Fraction (X)	pph (g/100g)
methanol	0.36	0.02	26.66

Ugi product 109C(UC) $C_{28}H_{30}F_3N_3O_5$ ⁶⁵



Compound Data

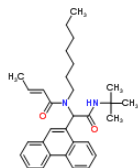
Molecular weight	545.55	H bond acceptors	8	Rule of 5 violations	1
Compound type	Ugi Product	H bond donors	2	ACD/ALogP	5
Phase 25°C	solid	Rotatable bonds	11	Predicted density	1.263 g/cm ³
SMILES	<chem>O=C(CNC(=O)OC(C)(C)C)N(Cc1ccc(oc1C(F)(F)F)C(c2ccccc2)C(=O)NCc3ccccc3</chem>				
InChIKey	<chem>XRHBVZVCUGMHPN-UHFFFAOYSA-N</chem>				

Solubility Data

Solvent	Concentration	Mole Fraction (X)	pph (g/100g)
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	(M)		
methanol	0.15	0.01	11.62

Ugi product 148B C₃₁H₄₀N₂O₂^{145, 96}



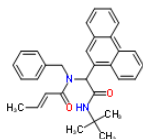
Compound Data

Molecular weight	472.661	H bond acceptors	4	Rule of 5 violations	1
Compound type	Ugi Product	H bond donors	1	ACD/ALogP	7.47
Phase 25°C	solid	Rotatable bonds	11	Predicted density	1.067 g/cm ³
SMILES	<chem>CC(C)(C)NC(=O)C(N(CCCCCC)C(=O))C=C(C)c2cc3ccccc3c1ccccc12</chem>				
InChIKey	HOKCUULFCASAQT-FRKPEAEDSA-N				

Solubility Data

Solvent	Concentration (M)	Mole Fraction (X)	pph (g/100g)
acetonitrile	0.02	0.00	1.28
benzene	0.05	0.00	2.77
ethanol	0.00	0.00	0.00
methanol	0.03	0.00	1.91
THF	0.40	0.04	25.03
toluene	0.14	0.02	8.10

Ugi product 150D(UC) C₃₁H₃₂N₂O₂^{78, 65}



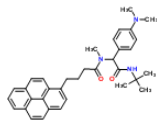
Compound Data

Molecular weight	464.598	H bond acceptors	4	Rule of 5 violations	1
Compound type	Ugi Product	H bond donors	1	ACD/ALogP	6.18
Phase 25°C	solid	Rotatable bonds	7	Predicted density	1.148 g/cm ³
SMILES	<chem>CC(C)(C)NC(=O)C(N(Cc1ccccc1)C(=O))C=C(C)c3cc4ccccc4c2ccccc23</chem>				
InChIKey	PBZQTKRWYXTXIS-WLRTZDKTSA-N				

Solubility Data

Solvent	Concentration (M)	Mole Fraction (X)	pph (g/100g)
acetonitrile	0.04	0.00	2.53
DMSO	0.18	0.01	8.21
ethanol	0.04	0.00	2.42
methanol	0.07	0.00	4.12
THF	0.49	0.05	31.41
toluene	0.04	0.00	2.17

Ugi product 171K (UC) C₃₅H₃₉N₃O₂⁶⁵



Compound Data

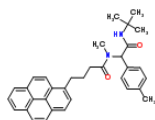
Molecular weight	533.703	H bond acceptors	5	Rule of 5 violations	2
Compound type	Ugi Product	H bond donors	1	ACD/ALogP	6.83
Phase 25°C	solid	Rotatable bonds	9	Predicted density	1.177 g/cm ³
SMILES	<chem>CN(C)c1ccc(cc1)C(C(=O)NC(C)(C)C)N(C)C(=O)CCCc5ccc4ccc3cccc2ccc5c4c23</chem>				
InChIKey	XWJCEFGKUMNBLK-UHFFFAOYSA-N				

Solubility Data

Solvent	Concentration (M)	Mole Fraction (X)	pph (g/100g)
methanol	0.02	0.00	1.43

Ugi product 173B (UC) C₃₄H₃₆N₂O₂⁶⁵

Compound Data

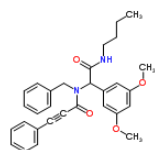


Molecular weight	504.662	H bond acceptors	4	Rule of 5 violations	2
Compound type	Ugi Product	H bond donors	1	ACD/ALogP	7.18
Phase 25°C	solid	Rotatable bonds	8	Predicted density	1.169 g/cm ³
SMILES	<chem>CC(C)(C)NC(=O)C(N(C)C(=O)CCCc4ccc3ccc2cccc1ccc4c3c12)c5ccc(C)cc5</chem>				
InChIKey	KNHNINYGWDFMQZ-UHFFFAOYSA-N				

Solubility Data

Solvent	Concentration (M)	Mole Fraction (X)	pph (g/100g)
methanol	0.08	0.00	5.55

Ugi product 173G (UC) C₃₀H₃₂N₂O₄⁶⁵



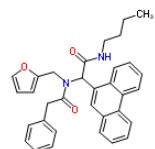
Compound Data

Molecular weight	484.586	H bond acceptors	6	Rule of 5 violations	1
Compound type	Ugi Product	H bond donors	1	ACD/ALogP	6.39
Phase 25°C	solid	Rotatable bonds	11	Predicted density	1.19 g/cm ³
SMILES	<chem>COc1cc(cc(OC)c1)C(C(=O)NCCCC)N(Cc2ccccc2)C(=O)C#Cc3ccccc3</chem>				
InChIKey	VOGZWAORWZGOTE-UHFFFAOYSA-N				

Solubility Data

Solvent	Concentration (M)	Mole Fraction (X)	pph (g/100g)
methanol	0.18	0.01	12.50

Ugi product 176C (UC) C₃₃H₃₂N₂O₃^{155, 127, 144}



Compound Data

Molecular weight	504.619	H bond acceptors	5	Rule of 5 violations	2
Compound type	Ugi Product	H bond donors	1	ACD/ALogP	6.9
Phase 25°C	solid	Rotatable bonds	10	Predicted density	1.197 g/cm ³
SMILES	<chem>O=C(Cc1ccccc1)N(Cc2ccco2)C(c4cc5ccccc5c3ccccc34)C(=O)NCCCC</chem>				
InChIKey	RGYLRDGAJICY-UHFFFAOYSA-N				

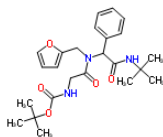
Solubility Data

Solvent	Concentration (M)	Mole Fraction (X)	pph (g/100g)
1-octanol	0.01	0.00	0.62
1,4-dioxane	0.19	0.02	10.47
acetonitrile	0.02	0.00	1.36
benzene	0.03	0.00	1.76
diethyl ether	0.02	0.00	1.39
DMF	0.27	0.02	17.67
DMSO	0.19	0.01	9.48
ethanol	0.01	0.00	0.65
methanol	0.02	0.00	1.35
THF	0.28	0.02	17.72
toluene	0.03	0.00	1.76

Ugi product 206B(UC) C₂₄H₃₃N₃O₅⁵⁶

Compound Data

Molecular weight	443.536	H bond acceptors	8	Rule of 5 violations	0
Compound type	Ugi Product	H bond donors	2	ACD/ALogP	3.74
Phase 25°C	solid	Rotatable bonds	10	Predicted density	1.145 g/cm ³
SMILES	<chem>O=C(CNC(=O)OC(C)(C)C)N(Cc1ccccc1)C(c2ccccc2)C(=O)NC(C)(C)C</chem>				



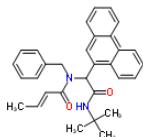
InChIKey

BXAOUWIVXLQYOZ-UHFFFAOYSA-N

Solubility Data

Solvent	Concentration (M)	Mole Fraction (X)	pph (g/100g)
2-propanol	0.00	0.00	0.00
acetonitrile	0.02	0.00	1.20
benzene	0.01	0.00	0.51
carbon tetrachloride	0.00	0.00	0.00
chloroform	0.57	0.06	21.63
cyclohexane	0.00	0.00	0.00
cyclopentane	0.00	0.00	0.00
dichloromethane	0.24	0.02	9.37
diethyl ether	0.00	0.00	0.00
DMF	0.24	0.02	13.49
DMSO	0.23	0.02	10.19
ethanol	0.02	0.00	1.15
hexane	0.00	0.00	0.00
methanol	0.05	0.00	3.00
THF	0.26	0.02	14.19
toluene	0.01	0.00	0.51

Ugi product 214C(UC) C₃₁H₃₂N₂O₂²⁷



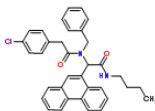
Compound Data

Molecular weight	464.598	H bond acceptors	4	Rule of 5 violations	1
Compound type	Ugi Product	H bond donors	1	ACD/ALogP	6.18
Phase 25°C	solid	Rotatable bonds	7	Predicted density	1.148 g/cm ³
SMILES	<chem>CC(C)(C)NC(=O)C(N(Cc1ccccc1)C(=O)C=C(C)c3cc4ccccc4c2ccccc23</chem>				
InChIKey	PBZQTKRWYXTXIS-WLRTZDKTSA-N				

Solubility Data

Solvent	Concentration (M)	Mole Fraction (X)	pph (g/100g)
methanol	0.01	0.00	0.62
THF	0.35	0.03	20.96

Ugi product 215F(UC) C₃₅H₃₃ClN₂O₂⁷¹



Compound Data

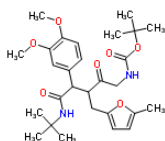
Molecular weight	549.102	H bond acceptors	4	Rule of 5 violations	2
Compound type	Ugi Product	H bond donors	1	ACD/ALogP	8.33
Phase 25°C	solid	Rotatable bonds	10	Predicted density	1.219 g/cm ³
SMILES	<chem>Clc5ccc(CC(=O)N(Cc1ccccc1)C(c3cc4ccccc4c2ccccc23)C(=O)NCCCC)cc5</chem>				
InChIKey	NCOSMKWGNCPJPCR-UHFFFAOYSA-N				

Solubility Data

Solvent	Concentration (M)	Mole Fraction (X)	pph (g/100g)
acetonitrile	0.04	0.00	2.99
DMSO	0.38	0.03	22.91
ethanol	0.06	0.00	4.34
methanol	0.12	0.01	9.25
THF	0.61	0.06	51.09

toluene	0.07	0.01	4.56
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Ugi Product 216-4A C₂₈H₄₀N₂O₇^{97, 93}

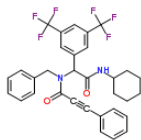


Compound Data					
Molecular weight	516.626	H bond acceptors	9	Rule of 5 violations	1
Compound type	Ugi Product	H bond donors	2	ACD/ALogP	4.08
Phase 25°C	solid	Rotatable bonds	13	Predicted density	1.12 g/cm ³
SMILES	<chem>Cc1ccc(o1)CC(C(c2ccc(c(c2)OC)OC)C(=O)NC(C)(C)C)C(=O)CNC(=O)OC(C)(C)C</chem>				
InChIKey					

Solubility Data

Solvent	Concentration (M)	Mole Fraction (X)	pph (g/100g)
acetonitrile	0.13	0.01	9.17
DMSO	0.06	0.00	2.90
ethanol	0.07	0.00	4.79
methanol	0.18	0.01	13.47
toluene	0.20	0.02	13.07

Ugi product 234 C₃₂H₂₈F₆N₂O₂⁶⁵

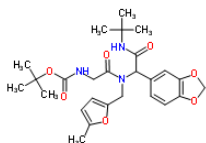


Compound Data					
Molecular weight	586.57	H bond acceptors	4	Rule of 5 violations	2
Compound type	Ugi Product	H bond donors	1	ACD/ALogP	8.56
Phase 25°C	solid	Rotatable bonds	7	Predicted density	1.33 g/cm ³
SMILES	<chem>c1ccc(cc1)CN(C(c2cc(cc(c2)C(F)(F)F)C(F)(F)F)C(=O)NC3CCCCC3)C(=O)C</chem> <chem>#Cc4ccccc4</chem>				
InChIKey					

Solubility Data

Solvent	Concentration (M)	Mole Fraction (X)	pph (g/100g)
ethanol	0.23	0.01	19.25

Ugi product 62E (UC) C₂₆H₃₅N₃O₇⁶⁵



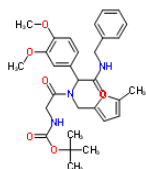
Compound Data					
Molecular weight	501.572	H bond acceptors	10	Rule of 5 violations	2
Compound type	Ugi Product	H bond donors	2	ACD/ALogP	4.06
Phase 25°C	solid	Rotatable bonds	10	Predicted density	1.209 g/cm ³
SMILES	<chem>CC(C)(C)NC(=O)C(c1ccc2OCOc2c1)N(Cc3ccc(C)o3)C(=O)CNC(=O)OC(C)(C)C</chem>				
InChIKey	MTSJLRXXXJHLDI-UHFFFAOYSA-N				

Solubility Data

Solvent	Concentration (M)	Mole Fraction (X)	pph (g/100g)
methanol	0.13	0.01	9.15

Ugi product 64C (UC) C₃₀H₃₇N₃O₇⁶⁵

Compound Data					
Molecular weight	551.631	H bond acceptors	10	Rule of 5 violations	2
Compound type	Ugi Product	H bond donors	2	ACD/ALogP	4.63

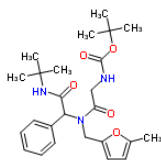


Phase 25°C	solid	Rotatable bonds	13	Predicted density	1.192 g/cm ³
SMILES	<chem>CC(C)(C)OC(=O)NCC(=O)N(Cc1ccc(C)o1)C(C(=O)NCc2ccccc2)c3ccc(OC)c(OC)c3</chem>				
InChIKey	VMMFSZQZVZNXXSK-UHFFFAOYSA-N				

Solubility Data

Solvent	Concentration (M)	Mole Fraction (X)	pph (g/100g)
methanol	0.03	0.00	2.23

Ugi product 86B (UC) C₂₅H₃₅N₃O₅⁶⁵



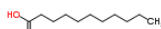
Compound Data

Molecular weight	457.562	H bond acceptors	8	Rule of 5 violations	0
Compound type	Ugi Product	H bond donors	2	ACD/ALogP	4.2
Phase 25°C	solid	Rotatable bonds	10	Predicted density	1.133 g/cm ³
SMILES	<chem>O=C(CNC(=O)OC(C)(C)N(Cc1ccc(C)o1)C(c2ccccc2)C(=O)NC(C)(C)C</chem>				
InChIKey	WDAGUORBKBNETC-UHFFFAOYSA-N				

Solubility Data

Solvent	Concentration (M)	Mole Fraction (X)	pph (g/100g)
methanol	0.17	0.01	11.09

undecanoic acid C₁₁H₂₂O₂⁵⁸



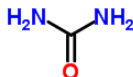
Compound Data

Molecular weight	186.291	H bond acceptors	2	Rule of 5 violations	0
Compound type	carboxylic acid	H bond donors	1	ACD/ALogP	4.5
Phase 25°C	solid	Rotatable bonds	9	Predicted density	0.909 g/cm ³
SMILES	<chem>O=C(O)CCCCCCCCC</chem>				
InChIKey	ZDPHROEEEOARMN-UHFFFAOYSA-N				

Solubility Data

Solvent	Concentration (M)	Mole Fraction (X)	pph (g/100g)
ethanol	3.94	0.55	488.75
methanol	4.00	0.49	549.05

urea CH₄N₂O⁵³



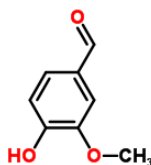
Compound Data

Molecular weight	60.0553	H bond acceptors	3	Rule of 5 violations	0
Compound type	amide	H bond donors	4	ACD/ALogP	-2.11
Phase 25°C	solid	Rotatable bonds	0	Predicted density	1.212 g/cm ³
SMILES	<chem>NC(=O)N</chem>				
InChIKey	XSQUKJJFZCRTK-UHFFFAOYSA-N				

Solubility Data

Solvent	Concentration (M)	Mole Fraction (X)	pph (g/100g)
methanol	2.66	0.12	24.44

vanillin C₈H₈O₃^{906, 4, 55, 11, 10, 207, 19}



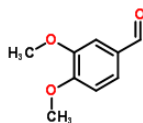
Compound Data

Molecular weight	152.147	H bond acceptors	3	Rule of 5 violations	0
Compound type	aldehyde	H bond donors	1	ACD/ALogP	1.19
Phase 25°C	solid	Rotatable bonds	3	Predicted density	1.231 g/cm ³
SMILES	<chem>Oc1ccc(cc1OC)C=O</chem>				
InChIKey	MWOOGOJBHIARFG-UHFFFAOYSA-N				

Solubility Data

Solvent	Concentration (M)	Mole Fraction (X)	pph (g/100g)
1-propanol	1.82	0.15	44.94
1,2-dichloroethane	1.17	0.10	17.74
acetonitrile	2.36	0.15	67.86
butanone	2.14	0.21	56.32
ethanol	2.47	0.17	69.35
methanol	4.16	0.27	173.01
THF	3.59	0.34	108.89
toluene	0.30	0.03	5.44

veratraldehyde C₉H₁₀O₃^{41, 71, 208}



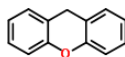
Compound Data

Molecular weight	166.174	H bond acceptors	3	Rule of 5 violations	0
Compound type	aldehyde	H bond donors	0	ACD/ALogP	1.61
Phase 25°C	solid	Rotatable bonds	3	Predicted density	1.114 g/cm ³
SMILES	<chem>COc1cc(ccc1OC)C=O</chem>				
InChIKey	WJUFSDZVCOTFON-UHFFFAOYSA-N				

Solubility Data

Solvent	Concentration (M)	Mole Fraction (X)	pph (g/100g)
acetone	3.03	0.29	119.01
acetonitrile	5.76	0.69	904.54
chloroform	5.70	0.75	421.71
dichloromethane	6.06	0.81	837.51
diethyl ether	3.55	0.43	170.84
DMSO	5.31	0.64	386.17
ethanol	5.49	0.64	645.97
hexane	0.07	0.01	1.74
methanol	5.87	0.67	1041.50
THF	5.33	0.68	480.29
toluene	4.54	0.60	267.44

xanthene C₁₃H₁₀O⁹⁰⁵



Compound Data

Molecular weight	182.218	H bond acceptors	1	Rule of 5 violations	0
Compound type	non-Ugi related	H bond donors	0	ACD/ALogP	3.93
Phase 25°C	solid	Rotatable bonds	0	Predicted density	1.159 g/cm ³
SMILES	<chem>O2c1ccccc1Cc3c2ccccc3</chem>				
InChIKey	GJCOSYZMQJWQCA-UHFFFAOYSA-N				

Solubility Data

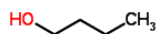
Solvent	Concentration (M)	Mole Fraction (X)	pph (g/100g)
1-butanol	0.19	0.02	4.43
1-decanol	0.24	0.05	5.49
1-heptanol	0.23	0.03	5.30
1-hexanol	0.22	0.03	5.09

1-octanol	0.24	0.04	5.52
1-pentanol	0.20	0.02	4.64
1-propanol	0.15	0.01	3.52
1,2-dichloroethane	1.62	0.15	33.77
2-butanol	0.13	0.01	3.02
2-methyl-1-pentanol	0.16	0.02	3.67
2-methyl-1-propanol	0.12	0.01	2.78
2-methyl-2-butanol	0.18	0.02	4.16
2-methyl-2-propanol	0.12	0.01	2.77
2-pentanol	0.16	0.02	3.70
2-propanol	0.11	0.01	2.58
2,2,4-trimethylpentane	0.15	0.02	3.95
3-methyl-1-butanol	0.15	0.02	3.46
4-methyl-2-pentanol	0.14	0.02	3.22
acetonitrile	0.35	0.02	9.03
carbon tetrachloride	1.25	0.12	16.71
cyclohexane	0.39	0.04	9.58
cyclooctane	0.38	0.05	9.32
cyclopentanol	0.33	0.03	6.32
decane	0.24	0.05	6.19
dibutyl ether	0.50	0.08	12.68
diethyl ether	0.79	0.08	22.39
diisopropyl ether	0.41	0.06	10.54
ethanol	0.10	0.01	2.37
heptane	0.24	0.03	6.54
hexadecane	0.24	0.07	5.88
hexane	0.23	0.03	6.44
methanol	0.10	0.00	2.46
methyl tert-butyl ether	0.65	0.08	17.59
methylcyclohexane	0.33	0.04	8.17
nonane	0.24	0.04	6.28
octane	0.25	0.04	6.67
undecane	0.23	0.05	5.85

Solvents

Below we present data for the solvents used in the Open Notebook Science Challenge. We present various properties such as density and boiling point together with important solvation related parameters such as dielectric constants and dipole moments [1000-1100].

1-butanol



Compound Data

Molecular weight	74.1216
Predicted density	0.805 g/cm ³
Boiling point	117.7 °C
Dipole moment	1.66
Dielectric constant	17.8
SMILES	CCCCO
InChIKey	LRHPLDYGVMQRHN-UHFFFAOYSA-N

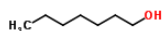
1-decanol



Compound Data

Molecular weight	158.2811
Predicted density	0.828 g/cm ³
Boiling point	227.8 °C
SMILES	OCCCCCCCCC
InChIKey	MWKFXSUHTGQN-UHFFFAOYSA-N

1-heptanol



Compound Data

Molecular weight	116.2013
Predicted density	0.82 g/cm ³
Boiling point	176.9 °C
SMILES	OCCCCCC
InChIKey	BBMCTIGTTCKYKF-UHFFFAOYSA-N

1-hexanol



Compound Data

Molecular weight	102.1748
Predicted density	0.816 g/cm ³
Boiling point	158.2 °C
Dipole moment	1.55
Dielectric constant	13.3
SMILES	OCCCCC
InChIKey	ZSIAUFGUXNUGDI-UHFFFAOYSA-N

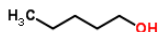
1-octanol



Compound Data

Molecular weight	130.2279
Predicted density	0.823 g/cm ³
Boiling point	194.7 °C
SMILES	OCCCCCCC
InChIKey	KBPLFHHGFOOTCA-UHFFFAOYSA-N

1-pentanol

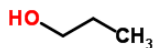


Compound Data

Molecular weight	88.1482
Predicted density	0.811 g/cm ³
Boiling point	138.5 °C
SMILES	OCCCC
InChIKey	AMQJEAYHLZJPGS-UHFFFAOYSA-N

1-propanol

Compound Data



Molecular weight	60.095
Predicted density	0.795 g/cm ³
Boiling point	95.8 °C
Dipole moment	1.68
Dielectric constant	20.1
SMILES	CCCO
InChIKey	BDERNNFJNOPAEC-UHFFFAOYSA-N

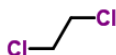
1,1,2-trichlorotrifluoroethane



Compound Data

Molecular weight	187.3756
Predicted density	1.67 g/cm ³
Boiling point	50.9 °C
SMILES	ClC(F)(F)C(Cl)(Cl)F
InChIKey	AJDIZQLSFPQPEY-UHFFFAOYSA-N

1,2-dichloroethane



Compound Data

Molecular weight	98.9592
Predicted density	1.173 g/cm ³
Boiling point	83.5 °C
SMILES	ClCCCl
InChIKey	WSLDOOZREJYCGB-UHFFFAOYSA-N

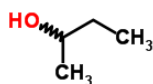
1,4-dioxane



Compound Data

Molecular weight	88.1051
Predicted density	0.995 g/cm ³
Boiling point	102.9 °C
SMILES	O1CCOCC1
InChIKey	RYHBNJHYFVUHQT-UHFFFAOYSA-N

2-butanol



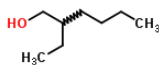
Compound Data

Molecular weight	74.1216
Predicted density	0.801 g/cm ³
Boiling point	96.6 °C
SMILES	OC(C)CC
InChIKey	BTANRVKWNQVYAZ-UHFFFAOYSA-N

2-ethyl-1-hexanol

Compound Data

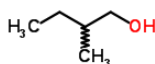
Molecular weight	130.2279
Predicted density	0.821 g/cm ³



Boiling point	184.6 °C
SMILES	<chem>OCC(CC)CCCC</chem>
InChIKey	YIWUKEYIRIRTPP-UHFFFAOYSA-N

2-methyl-1-butanol

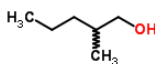
Compound Data



Molecular weight	88.1482
Predicted density	0.809 g/cm ³
Boiling point	128.7 °C
SMILES	<chem>OCC(C)CC</chem>
InChIKey	QPRQEDXDYOZYLA-UHFFFAOYSA-N

2-methyl-1-pentanol

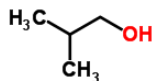
Compound Data



Molecular weight	102.1748
Predicted density	0.814 g/cm ³
Boiling point	148 °C
SMILES	<chem>OCC(C)CCC</chem>
InChIKey	PFNHSEQQEPMLNI-UHFFFAOYSA-N

2-methyl-1-propanol

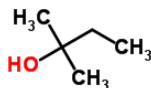
Compound Data



Molecular weight	74.1216
Predicted density	0.801 g/cm ³
Boiling point	105 °C
SMILES	<chem>OCC(C)C</chem>
InChIKey	ZXEKIIBDNHEJCQ-UHFFFAOYSA-N

2-methyl-2-butanol

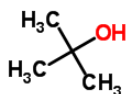
Compound Data



Molecular weight	88.1482
Predicted density	0.811 g/cm ³
Boiling point	102 °C
SMILES	<chem>OC(C)(C)CC</chem>
InChIKey	MSXVEPNJUHWWQHW-UHFFFAOYSA-N

2-methyl-2-propanol

Compound Data

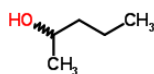


Molecular weight	74.1216
Predicted density	0.804 g/cm ³
Boiling point	84.6 °C
SMILES	<chem>OC(C)(C)C</chem>

InChIKey

DKGAVHZHDRPRBM-UHFFFAOYSA-N

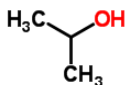
2-pentanol



Compound Data

Molecular weight	88.1482
Predicted density	0.809 g/cm ³
Boiling point	118.8 °C
SMILES	<chem>OC(C)CCC</chem>
InChIKey	JYVLIDXNZAXMDK-UHFFFAOYSA-N

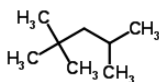
2-propanol



Compound Data

Molecular weight	60.095
Predicted density	0.791 g/cm ³
Boiling point	73 °C
Dipole moment	1.66
Dielectric constant	1.89
SMILES	<chem>CC(O)C</chem>
InChIKey	KFZMGEQAYNKOFK-UHFFFAOYSA-N

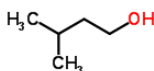
2,2,4-trimethylpentane



Compound Data

Molecular weight	114.2285
Predicted density	0.709 g/cm ³
Boiling point	98.8 °C
SMILES	<chem>CC(C)CC(C)(C)C</chem>
InChIKey	NHTMVDHEPJAVLT-UHFFFAOYSA-N

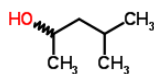
3-methyl-1-butanol



Compound Data

Molecular weight	88.1482
Predicted density	0.809 g/cm ³
Boiling point	131.2 °C
SMILES	<chem>OCCC(C)C</chem>
InChIKey	PHTQWCKDNZKARW-UHFFFAOYSA-N

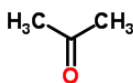
4-methyl-2-pentanol



Compound Data

Molecular weight	102.1748
Predicted density	0.811 g/cm ³
Boiling point	133.5 °C
SMILES	<chem>OC(C)CC(C)C</chem>
InChIKey	WVYWICLMDOOCFB-UHFFFAOYSA-N

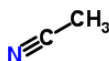
acetone



Compound Data

Molecular weight	58.0791
Predicted density	0.772 g/cm ³
Boiling point	46.5 °C
Dipole moment	2.88
Dielectric constant	20.7
SMILES	CC(=O)C
InChIKey	CSCPPACGZOOCGX-UHFFFAOYSA-N

acetonitrile



Compound Data

Molecular weight	41.0519
Predicted density	0.747 g/cm ³
Boiling point	63.5 °C
Dipole moment	3.92
Dielectric constant	36.6
SMILES	CCN
InChIKey	QUSNBJAOMFDIB-UHFFFAOYSA-N

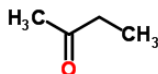
benzene



Compound Data

Molecular weight	78.1118
Predicted density	0.873 g/cm ³
Boiling point	78.8 °C
Dipole moment	0
Dielectric constant	2.28
SMILES	c1ccccc1
InChIKey	UHOVQNZJYSORNB-UHFFFAOYSA-N

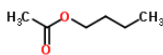
butanone



Compound Data

Molecular weight	72.1057
Predicted density	0.786 g/cm ³
Boiling point	75.6 °C
SMILES	CC(=O)CC
InChIKey	ZWEHNKRNPQVVGH-UHFFFAOYSA-N

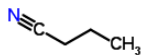
butyl acetate



Compound Data

Molecular weight	116.1583
Predicted density	0.886 g/cm ³
Boiling point	126.6 °C
SMILES	CC(=O)OCCCC
InChIKey	DKPFZGUDAPQIHT-UHFFFAOYSA-N

butyronitrile



Compound Data

Molecular weight	69.1051
Predicted density	0.785 g/cm ³
Boiling point	117.3 °C
SMILES	N#CCCC
InChIKey	KVNRLNFWIYMESJ-UHFFFAOYSA-N

carbon disulfide



Compound Data

Molecular weight	76.1407
Predicted density	1.259 g/cm ³
Boiling point	46.2 °C
SMILES	S=C=S
InChIKey	QGGJOPFRUJISHPQ-UHFFFAOYSA-N

carbon tetrachloride



Compound Data

Molecular weight	153.8227
Predicted density	1.697 g/cm ³
Boiling point	76 °C
Dipole moment	0
Dielectric constant	2.24
SMILES	[C](Cl)(Cl)(Cl)Cl
InChIKey	VZGDMQKNWNREIO-UHFFFAOYSA-N

chloroform



Compound Data

Molecular weight	119.3776
Predicted density	1.5 g/cm ³
Boiling point	61.2 °C
Dipole moment	1.15
Dielectric constant	5.5
SMILES	C(Cl)(Cl)Cl
InChIKey	HEDRZPFGACZZDS-UHFFFAOYSA-N

cyclohexane



Compound Data

Molecular weight	84.1595
Predicted density	0.79 g/cm ³
Boiling point	80.7 °C
Dipole moment	0
Dielectric constant	18.5
SMILES	C1CCCCC1
InChIKey	XDTMQSROBMDMFD-UHFFFAOYSA-N

cyclooctane



Compound Data

Molecular weight	112.2126
Predicted density	0.79 g/cm ³
Boiling point	152 °C
SMILES	C1CCCCCCC1
InChIKey	WJTCGQSWYFHTAC-UHFFFAOYSA-N

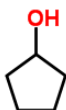
cyclopentane



Compound Data

Molecular weight	70.1329
Predicted density	0.79 g/cm ³
Boiling point	49.2 °C
SMILES	C1CCCC1
InChIKey	RGSFGYAAUTVSQA-UHFFFAOYSA-N

cyclopentanol



Compound Data

Molecular weight	86.1323
Predicted density	1.004 g/cm ³
Boiling point	140.8 °C
SMILES	OC1CCCC1
InChIKey	XCIXKGXIYUWCLL-UHFFFAOYSA-N

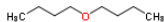
decane



Compound Data

Molecular weight	142.2817
Predicted density	0.734 g/cm ³
Boiling point	174.9 °C
SMILES	C(CCCCCCCC)C
InChIKey	DIOQZVSQGTUSAI-UHFFFAOYSA-N

dibutyl ether



Compound Data

Molecular weight	130.2279
Predicted density	0.78 g/cm ³
Boiling point	142.1 °C
SMILES	O(CCCC)CCCC
InChIKey	DURPTKYDGMSBL-UHFFFAOYSA-N

dichloromethane

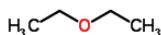
Compound Data

Molecular weight	84.9326
Predicted density	1.252 g/cm ³
Boiling point	39.6 °C



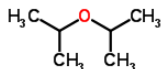
Dipole moment	1.6
Dielectric constant	9.08
SMILES	<chem>C(Cl)Cl</chem>
InChIKey	YMWUJEATGCHHMB-UHFFFAOYSA-N

diethyl ether



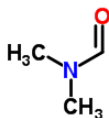
Compound Data	
Molecular weight	74.1216
Predicted density	0.734 g/cm ³
Boiling point	33.2 °C
Dipole moment	1.15
Dielectric constant	4.34
SMILES	<chem>CCOCC</chem>
InChIKey	RTZKZFJDLAIFYH-UHFFFAOYSA-N

diisopropyl ether



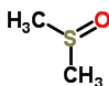
Compound Data	
Molecular weight	102.1748
Predicted density	0.758 g/cm ³
Boiling point	68.3 °C
SMILES	<chem>CC(C)OC(C)C</chem>
InChIKey	ZAFNJMIOTHYJRJ-UHFFFAOYSA-N

DMF



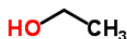
Compound Data	
Molecular weight	73.0938
Predicted density	0.87 g/cm ³
Boiling point	153 °C
Dipole moment	3.82
Dielectric constant	38.3
SMILES	<chem>O=C(NC)C</chem>
InChIKey	OHLUHNLEMFGTQ-UHFFFAOYSA-N

DMSO



Compound Data	
Molecular weight	78.1334
Predicted density	1.099 g/cm ³
Boiling point	189 °C
Dipole moment	3.96
Dielectric constant	47.2
SMILES	<chem>CS(=O)C</chem>
InChIKey	IAZDPXIMUYVGZ-UHFFFAOYSA-N

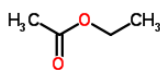
ethanol



Compound Data

Molecular weight	46.0684
Predicted density	0.78 g/cm ³
Boiling point	72.6 °C
Dipole moment	1.69
Dielectric constant	24.3
SMILES	CCO
InChIKey	LFQSCWFLJHTTHZ-UHFFFAOYSA-N

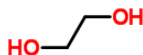
ethyl acetate



Compound Data

Molecular weight	88.1051
Predicted density	0.898 g/cm ³
Boiling point	73.9 °C
Dipole moment	1.78
Dielectric constant	6.02
SMILES	CCOC(=O)C1=NN(C(=N1)C(Cl)(Cl)Cl)C2=C(C(C=C2)Cl)Cl
InChIKey	GMBRUAIJFRHFQ-UHFFFAOYSA-N

ethylene glycol



Compound Data

Molecular weight	62.0678
Predicted density	1.097 g/cm ³
Boiling point	197.5 °C
SMILES	OCCO
InChIKey	LYCAIKOWRPUZTN-UHFFFAOYSA-N

heptane



Compound Data

Molecular weight	100.2019
Predicted density	0.695 g/cm ³
Boiling point	98.8 °C
SMILES	CCCCCCC
InChIKey	IMNFDUFMRHMDMM-UHFFFAOYSA-N

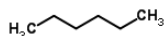
hexadecane



Compound Data

Molecular weight	226.4412
Predicted density	0.773 g/cm ³
Boiling point	286.6 °C
SMILES	CCCCCCCCCCCCCCCC
InChIKey	DCAYPVUWAIABOU-UHFFFAOYSA-N

hexane



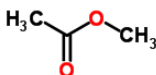
Compound Data	
Molecular weight	86.1754
Predicted density	0.675 g/cm ³
Boiling point	68.5 °C
Dipole moment	0.08
Dielectric constant	2.02
SMILES	CCCCCC
InChIKey	VLKZOEYAKHREP-UHFFFAOYSA-N

methanol



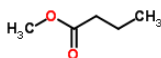
Compound Data	
Molecular weight	32.0419
Predicted density	0.753 g/cm ³
Boiling point	48.1 °C
Dipole moment	1.7
Dielectric constant	33
SMILES	CO
InChIKey	OKKJLVBELUTLKV-UHFFFAOYSA-N

methyl acetate



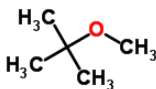
Compound Data	
Molecular weight	74.0785
Predicted density	0.908 g/cm ³
Boiling point	44 °C
SMILES	CC(=O)OC
InChIKey	KKKVLQRXCPHEJC-UHFFFAOYSA-N

methyl butyrate



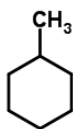
Compound Data	
Molecular weight	102.1317
Predicted density	0.891 g/cm ³
Boiling point	104.2 °C
SMILES	CCCC(=O)OC
InChIKey	UUIQMZJEGPQKFD-UHFFFAOYSA-N

methyl tert-butyl ether



Compound Data	
Molecular weight	88.1482
Predicted density	0.75 g/cm ³
Boiling point	55.2 °C
SMILES	CC(C)(C)OC
InChIKey	BZLVMXJERCZMT-UHFFFAOYSA-N

methylcyclohexane

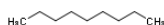


Compound Data

Molecular weight	98.1861
Predicted density	0.776 g/cm ³
Boiling point	101.1 °C
SMILES	CC1CCCCC1
InChIKey	UAEPNZWRGJTJPN-UHFFFAOYSA-N

nonane

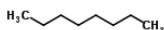
Compound Data



Molecular weight	128.2551
Predicted density	0.724 g/cm ³
Boiling point	151.7 °C
SMILES	CCCCCCCCC
InChIKey	BKIMMITUMNQMO5-UHFFFAOYSA-N

octane

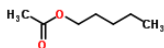
Compound Data



Molecular weight	114.2285
Predicted density	0.711 g/cm ³
Boiling point	126.4 °C
SMILES	CCCCCCCC
InChIKey	TVMXDCGIABBOFY-UHFFFAOYSA-N

pentyl acetate

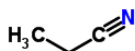
Compound Data



Molecular weight	130.1849
Predicted density	0.882 g/cm ³
Boiling point	149.9 °C
SMILES	CC(=O)OCCCCC
InChIKey	PGMYKACGE0XYJE-UHFFFAOYSA-N

propionitrile

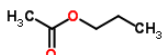
Compound Data



Molecular weight	55.0785
Predicted density	0.771 g/cm ³
Boiling point	91.3 °C
SMILES	CCC#N
InChIKey	FVSKHRXBFJPNKK-UHFFFAOYSA-N

propyl acetate

Compound Data

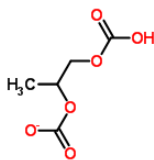


Molecular weight	102.1317
Predicted density	0.891 g/cm ³
Boiling point	101.4 °C
SMILES	CC(=O)OCCC

InChIKey

YKYONYBAUNKHLG-UHFFFAOYSA-N

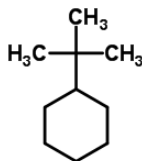
propylene carbonate



Compound Data

Molecular weight	163.106
Predicted density	1.205 g/cm ³
Boiling point	332.3 °C
SMILES	<chem>OC(=O)OCC(C)OC(=O)[O-]</chem>
InChIKey	ZEBXBLIKXVICMJ-UHFFFAOYSA-M

tert-butylcyclohexane



Compound Data

Molecular weight	140.2658
Predicted density	0.812 g/cm ³
Boiling point	168.3 °C
SMILES	<chem>CC(C)(C)C1CCCC1</chem>
InChIKey	XTVMZZBLCLWBPM-UHFFFAOYSA-N

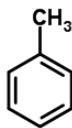
THF



Compound Data

Molecular weight	72.1057
Predicted density	0.904 g/cm ³
Boiling point	68.3 °C
Dipole moment	1.63
Dielectric constant	7.52
SMILES	<chem>C1CCOC1</chem>
InChIKey	WYURNTSHIVDZCO-UHFFFAOYSA-N

toluene



Compound Data

Molecular weight	92.1384
Predicted density	0.871 g/cm ³
Boiling point	110.6 °C
Dipole moment	0.36
Dielectric constant	2.38
SMILES	<chem>c1ccccc1C</chem>
InChIKey	YXFVVABEGXRONW-UHFFFAOYSA-N

undecane



Compound Data

Molecular weight	156.3083
Predicted density	0.743 g/cm ³
Boiling point	196.3 °C
SMILES	<chem>C(CCCCCCCC)CC</chem>
InChIKey	RSJKGSCJYJTIGS-UHFFFAOYSA-N

water

H₂O

Compound Data

Molecular weight	18.0153
Predicted density	0.998 g/cm ³
Boiling point	100 °C
SMILES	O
InChIKey	XYLOFNOQVPJJNP-UHFFFAOYSA-N

Table 1. Abraham solubility coefficients

Solvent	c	e	s	a	b	v
1-butanol	0.152	0.438	-1.177	0.096	-3.919	4.122
1-decanol	-0.062	0.754	-1.461	0.063	-4.053	4.293
1-heptanol	-0.026	0.491	-1.258	0.035	-4.155	4.415
1-hexanol	0.044	0.47	-1.153	0.083	-4.057	4.249
1-octanol	-0.034	0.489	-1.044	-0.024	-4.235	4.218
1-pentanol	0.08	0.521	-1.294	0.208	-3.908	4.208
1-propanol	0.148	0.436	-1.098	0.389	-3.893	4.036
1,2-dichloroethane	0.183	0.294	-0.134	-2.801	-4.291	4.18
1,4-dioxane	0.098	0.35	-0.083	-0.556	-4.826	4.172
2-butanol	0.194	0.383	-0.956	0.134	-3.606	3.829
2-methyl-1-propanol	0.161	0.31	-1.069	0.183	-3.774	4.04
2-methyl-2-propanol	0.197	0.136	-0.916	0.318	-4.031	4.112
2-pentanol	0.115	0.455	-1.331	0.206	-3.745	4.201
2-propanol	0.102	0.315	-1.02	0.532	-3.865	4.023
2,2,4-trimethylpentane	0.318	0.555	-1.737	-3.677	-4.864	4.417
3-methyl-1-butanol	0.123	0.37	-1.243	0.074	-3.781	4.208
acetone	0.313	0.312	-0.121	-0.608	-4.753	3.942
acetonitrile	0.413	0.077	0.326	-1.566	-4.391	3.364
benzene	0.142	0.464	-0.588	-3.009	-4.625	4.491
butanone	0.246	0.256	-0.08	-0.767	-4.855	4.148
butyl acetate	0.248	0.356	-0.501	-0.867	-4.973	4.281
carbon disulfide	0.047	0.686	-0.943	-3.603	-5.818	4.921
carbon tetrachloride	0.199	0.523	-1.159	-3.56	-4.594	4.618
chloroform	0.191	0.105	-0.403	-3.112	-3.514	4.395
cyclohexane	0.159	0.784	-1.678	-3.74	-4.929	4.577
decane	0.16	0.585	-1.734	-3.435	-5.078	4.582
dibutyl ether	0.203	0.369	-0.954	-1.488	-5.426	4.508
dichloromethane	0.319	0.102	-0.187	-3.058	-4.09	4.324
diethyl ether	0.33	0.401	-0.814	-0.457	-4.959	4.32
DMF	-0.305	-0.058	0.343	0.358	-4.865	4.486
DMSO	-0.194	0.327	0.791	1.26	-4.54	3.361
ethanol	0.208	0.409	-0.959	0.186	-3.645	3.928
ethyl acetate	0.328	0.369	-0.446	-0.7	-4.904	4.15
ethylene glycol	-0.243	0.695	-0.67	0.726	-2.399	2.67
heptane	0.325	0.67	-2.061	-3.317	-4.733	4.543
hexadecane	0.087	0.667	-1.617	-3.587	-4.869	4.433
hexane	0.361	0.579	-1.723	-3.599	-4.764	4.344
methanol	0.329	0.299	-0.671	0.08	-3.389	3.512
methyl acetate	0.351	0.223	-0.15	-1.035	-4.527	3.972
methyl tert-butyl ether	0.376	0.264	-0.788	-1.078	-5.03	4.41
methylcyclohexane	0.246	0.782	-1.982	-3.517	-4.293	4.528
nonane	0.24	0.619	-1.713	-3.532	-4.921	4.482
octane	0.223	0.642	-1.647	-3.48	-5.067	4.526
THF	0.207	0.372	-0.392	-0.236	-4.934	4.447
toluene	0.143	0.527	-0.72	-3.01	-4.824	4.545
undecane	0.058	0.603	-1.661	-3.421	-5.12	4.619

water	0	0	0	0	0	0
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Table 2. Hansen solubility parameters

Solvent	δ_d	δ_p	δ_h
1-butanol	16	5.7	15.8
1-decanol	17.5	2.6	10
1-heptanol	15.1	8	13
1-hexanol	14.1	8.6	12.7
1-octanol	17	3.3	11.9
1-pentanol	15.9	5.9	13.9
1-propanol	16	6.8	17.4
1,4-dioxane	19	1.8	7.4
2-butanol	15.8	5.7	14.5
2-methyl-1-butanol	16	5.1	14.3
2-methyl-1-propanol	15.1	5.7	15.9
2-methyl-2-propanol	15.2	5.1	14.7
2-pentanol	15.6	6.4	13.3
2-propanol	15.8	6.1	16.4
2,2,4-trimethylpentane	14.1	0	0
3-methyl-1-butanol	15.8	5.2	13.3
acetone	15.5	10.4	7
acetonitrile	15.3	18	6.1
benzene	18.4	0	2
butyl acetate	15.8	3.7	6.3
carbon tetrachloride	17.8	0	0.6
chloroform	17.8	3.1	5.7
cyclohexane	16.8	0	0.2
cyclooctane	17.5	0	0
cyclopentane	16.4	0	1.8
decane	15.7	0	0
dibutyl ether	15.7	4.5	4.2
dichloromethane	18.2	6.3	6.1
diethyl ether	14.5	2.9	5.1
DMF	17.4	16.7	11.3
DMSO	18.4	16.4	10.2
ethanol	15.8	8.8	19.4
ethyl acetate	15.8	5.3	7.2
ethylene glycol	17	11	26
heptane	15.3	0	0
hexadecane	16.3	0	0
hexane	14.9	0	0
methanol	15.1	12.3	22.3
methyl acetate	15.5	7.2	7.6
nonane	15.7	0	0
octane	15.5	0	0
propylene carbonate	20	18	4.1
THF	16.8	5.7	8
toluene	18	1.4	2
undecane	16	0	0

Solubility Modeling - Abraham General Solvation Model

Abraham Descriptors

Abraham *et al.*, have developed equations, the *Abraham solvation equations*, that can be used to predict the solubility of organic compounds in 84 different organic solvents [1]. The Abraham method assumes that the partition coefficient between water and a solvent, P_s , is given by the ratio of solubilities of a solute in the solvent, S_s , and in water, S_w ,

$$P_s = S_s / S_w. (1)$$

If this assumption is reasonable for the solute and solvent in question, then the solubility of the solute in the solvent can be calculated from the predicted partition coefficient,

$$\log S_s = \log S_w + c + e E + s S + a A + b B + v V, (2)$$

where the continually refined (as more experimental data becomes available) coefficients c, e, s, b, and v vary by solvent, see Table 1, and E, S, A, B, and V are solute descriptors, described as follows:

E is the solute **excess molar refractivity** in units of (cubic cm per mol)/10.

S is the solute **dipolarity/polarizability**.

A is the **overall (summation) hydrogen bond acidity**.

B is the **overall (summation) hydrogen bond basicity**.

V is the **McGowan characteristic volume** in units of (cubic cm per mol)/100.

Descriptor Calculation Methods

Various methods are used to determine the solute descriptors either from first principles or by working backwards from known logP and solubility values. Abraham *et al.* [2] have published a review of methods. The following sections detail the method used in this book to calculate the Abraham solute descriptors.

log S_w - The logarithm of the molar solubility in water

If the water solubility is known, then log S_w is simply the logarithm of this value. If the water solubility is not known, it can be approximated using the free web-service provided by VCCLab [<http://www.vccclab.org/web/alogps/>]. If the web service fails, the value can be approximated using the 1-octanol solubility via equation (1). If neither the water or the 1-octanol solubility is known, then log S_w is calculated using linear regression from all known solubility data, see S, A, and B below. If log S_w is predicted rather than measured, it will be italicized when presented.

V - The McGowan characteristic volume

V is the McGowan approximation for the molecular volume. It can be calculated from fragment contributions from the solute's molecular formula and the number of bonds. We calculated the McGowan volume from predicted values for the molar volume found on ChemSpider by using

$$V (\text{intrinsic}) = 0.597 + 0.6823 V. (3) [3]$$

E - The excess molar refractivity

E is the molar refraction, MR, of the compound calculated using McGowan's volume less the molar refraction of an alkane with the same McGowan volume,

$$E = (MR) - 2.83195 V + 0.52553, (4)$$

where

$$MR = 10 (\eta^2 - 1)/(\eta^2 + 2) V \text{ where } \eta \text{ is the refractive index. (5)}$$

We calculated the E from predicted values for MR (intrinsic) found on ChemSpider and by using

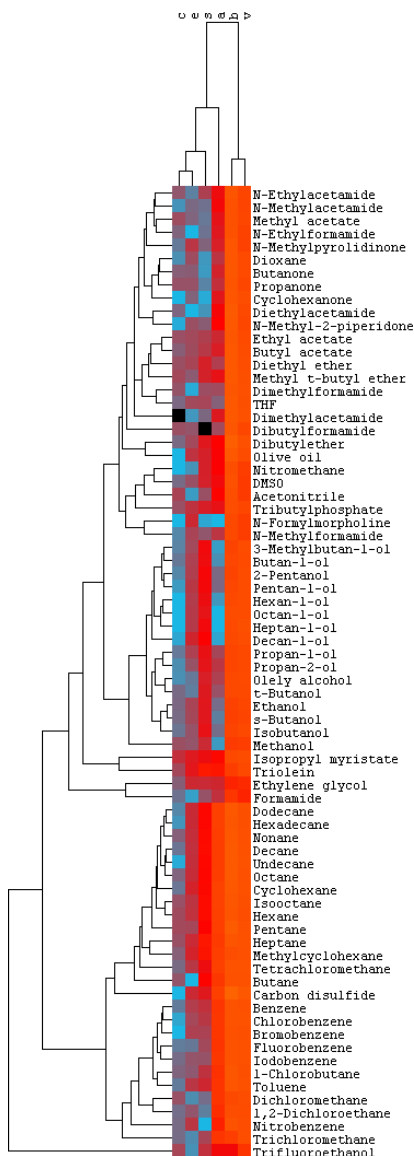
$$MR (\text{intrinsic}) = V (\text{intrinsic}) * MR / V (6).$$

S, A, and B

S, A, and B can be calculated from GLC [2], RP-HPLC [4], or simple linear regression from known solubility data or known logP values. We calculated S, A, and B by performing linear regression on the solutes with at least five solubility values in the Open Notebook Science Challenge database. When using the descriptors to predict the solubility of the solute in other organic solvents it is important to note that the more solvents used in the regression analysis, the more accurate the descriptors are likely to be. Solubility values for carboxylic acids in toluene or benzene were not used in the regression analysis since they are known to dimerize. Similarly, care must be taken when using Abraham descriptors to predict the solubility of carboxylic acids in toluene and benzene [5].

Clustering

By giving each solvent descriptors (c, e, s, a, b, v) it becomes possible to determine which solvents are similar by comparing their descriptors - much like as is done with Hansen solubility parameters. Using recently updated values [1], we used HappieClust to perform a cluster analysis (agglomerative hierarchical clustering) to see which solvents are considered similar in the Abraham general solvation method. The results are depicted in the figure below.



References

- [1] Abraham M.H.; Smith R.E.; Luchtefeld R.; Boorem A.J.; Luo R.; Acree Jr. W.E. Prediction of solubility of drugs and other compounds in organic solvents. *J. Pharm. Sci.* Early View Sept. 22 (2009) [<http://dx.doi.org/10.1002/jps.21922>]
- [2] Abraham M.H.; Ibrahim, A.; Zissimos, A.M. The determination of sets of solute descriptors from chromatographic measurements. *J Chromatogr. A* 1037(1-2):29–47 (2004) [<http://dx.doi.org/10.1016/j.chroma.2003.12.004>]
- [3] Abraham M.H.; McGowan J.C. The use of characteristic volumes to measure cavity terms in reversed phase liquid chromatography. *Chromatographia* 23(4) 243-246 (1987) [<http://dx.doi.org/10.1007/BF02311772>]
- [4] Andreas M.Z.; Abraham M.H.; Du C.M.; Valko K.; Bevan, C.; Reynolds, D.; Wood, J.; Tam, K.Y. Calculation of Abraham descriptors from experimental data from seven HPLC systems; evaluation of five different methods of calculation. *J. Chem. Soc. Perk. Trans. 2*. 2001-2010.(2002) [<http://dx.doi.org/10.1039/b206927j>]
- [5] Stovall D.M. Thermodynamics of the Abraham general solvation model: Solubility and partition aspects. Masters Thesis. University of Texas.(2006) [<http://digital.library.unt.edu/permalink/meta-dc-5342:1>]

Summary of Results

A summary of the results of the regression analyses giving the Abraham solute descriptors are presented below in Table 3.

Table 3. Abraham solute descriptors

Solute	E	S	A	B	V
1-octadecylamine	0.011	1.290	0.034	1.979	3.951
2-chloro-5-nitrobenzaldehyde	1.221	1.359	-0.054	0.182	0.954
2-chloro-5-nitrobenzoic acid	1.220	1.109	0.773	0.178	0.967
2-methoxybenzoic acid	0.850	1.328	0.422	0.477	0.970
2-methylbenzoic acid	0.854	0.689	0.368	0.284	0.857
2-phenylbutyric acid	0.878	1.077	0.009	0.583	1.332
4-acetamidobenzoic acid	1.279	1.112	0.793	0.734	1.104
4-chloro-3-nitrobenzoic acid	1.220	1.317	0.583	0.371	0.967
4-chlorobenzaldehyde	0.933	0.716	0.080	0.087	0.781
4-chlorophenylacetic acid	0.980	0.565	0.265	0.257	1.013
4-dimethylaminobenzaldehyde	1.190	1.602	0.079	0.756	1.162
4-fluorobenzoic acid	0.726	0.720	0.400	0.168	0.680
4-hydroxybenzaldehyde	0.918	1.003	0.439	0.225	0.583
4-methoxybenzoic acid	0.850	1.290	0.404	0.552	0.970
4-methoxyphenylacetic acid	0.877	1.137	0.101	0.678	1.189
4-nitrobenzaldehyde	1.049	1.634	-0.031	0.289	0.780
4-nitrobenzoic acid	1.048	1.301	0.518	0.349	0.793
4-phenylbutyric acid	0.896	3.980	0.540	-0.076	1.321
4-pyrenebutanoic acid	3.727	2.030	0.411	0.855	2.385
9-fluorenone	1.638	1.392	0.097	0.233	1.247
acetylsalicylic acid	0.946	5.432	0.815	-0.028	1.170
benzoic acid	0.788	0.144	0.100	0.239	0.618
boc-glycine	0.402	0.823	0.255	0.784	1.338
chloroacetic acid	0.502	0.372	0.096	0.042	0.114
cinnamic acid	1.161	4.115	0.445	-0.194	0.957
crotonic acid	0.474	0.405	0.130	0.155	0.339
diphenylacetic acid	1.565	1.499	0.147	1.083	1.773
furoic acid	0.590	0.351	0.479	0.125	0.366
ibuprofen	0.942	1.122	0.444	1.364	2.061
mandelic acid	0.970	6.447	1.008	-0.527	0.812
nicotinic acid	0.762	0.738	0.461	0.681	0.519
o-vanillin	1.024	0.802	0.046	0.448	0.935
phenanthrene	2.100	0.840	0.057	0.198	1.435
phenanthrene-9-carboxaldehyde	2.494	1.166	0.327	0.423	1.606
phenylacetic acid	0.832	0.917	0.082	0.455	0.837
piperonal	1.032	0.928	0.118	0.175	0.769
salicylic acid	0.920	0.110	0.410	0.111	0.595
thianthrene	2.281	1.312	-0.101	0.786	1.543
UCExp216-3A	2.332	4.791	-0.007	3.981	5.203
Ugi product 148B	3.440	5.683	0.240	3.436	5.615
Ugi product 150D(UC)	4.342	4.362	0.051	3.236	5.052
Ugi product 176C (UC)	4.713	4.490	0.151	3.935	5.298
Ugi product 206B(UC)	1.915	2.463	0.301	3.663	4.800
Ugi product 215F(UC)	5.307	4.975	0.047	3.742	5.726
Ugi Product 216-4A	1.716	4.742	-0.317	4.359	5.883
vanillin	1.024	1.086	0.365	0.411	0.935
veratraldehyde	0.889	1.091	0.204	0.572	1.310
xanthene	1.517	1.171	-0.085	0.454	1.428

Measured and predicted values

1-octadecylamine C₁₈H₃₉N - 6 solvents^{69, 908}

Compound Data

	Molecular weight 269.509	H bond acceptors 1	Rule of 5 violations 1
Compound type amine	H bond donors 2	ACD/ALogP 8.37	
Phase 25°C solid	Rotatable bonds 17	Predicted density 0.818 g/cm ³	
SMILES	NCCCCCCCCCCCCCCCCC		
InChIKey	REYJJPSVUYRZGE-UHFFFAOYSA-N		

Abraham Solute Descriptors

log S _w	E	S	A	B	V
-6.910	0.011	1.290	0.034	1.979	3.951

Solubility Data

Solvent	Concentration (M)		Solvent bp °C
	Measured	Predicted	
acetonitrile	0.08	0.03	63.5
ethanol	1.77	2.39	72.6
hexane	0.13	0.07	68.5
methanol	1.68	0.54	48.1
THF	1.68	3.91	68.3
toluene	1.34	4.14	110.6
1-butanol	-	1.83	117.7
1-decanol	-	1.24	227.8
1-heptanol	-	4.66	176.9
1-hexanol	-	2.59	158.2
1-octanol	-	1.00	194.7
1-pentanol	-	2.55	138.5
1-propanol	-	1.21	95.8
1,2-dichloroethane	-	> 9	83.5
1,4-dioxane	-	1.00	102.9
2-butanol	-	1.13	96.6
2-methyl-1-propanol	-	2.37	105.0
2-methyl-2-propanol	-	2.44	84.6
2-pentanol	-	4.87	118.8
2-propanol	-	1.39	73.0
2,2,4-trimethylpentane	-	0.07	98.8
3-methyl-1-butanol	-	5.75	131.2
acetone	-	0.25	46.5
benzene	-	> 9	78.8
butanone	-	0.98	75.6
butyl acetate	-	0.55	126.6
carbon disulfide	-	0.54	46.2
carbon tetrachloride	-	6.78	76.0
chloroform	-	> 9	61.2
cyclohexane	-	0.20	80.7
decane	-	0.09	174.9
dibutyl ether	-	0.12	142.1
dichloromethane	-	> 9	39.6
diethyl ether	-	0.41	33.2
DMF	-	> 9	153.0
DMSO	-	0.02	189.0
ethyl acetate	-	0.33	73.9
ethylene glycol	-	0.01	197.5
heptane	-	0.17	98.8
hexadecane	-	0.07	286.6
methyl acetate	-	0.89	44.0
methyl tert-butyl ether	-	0.77	55.2
methylcyclohexane	-	1.15	101.1
nonane	-	0.09	151.7
octane	-	0.09	126.4

undecane	-	0.10	196.3
water	-	0.00	100.0

2-chloro-5-nitrobenzaldehyde C₇H₄ClNO₃ - 5 solvents^{105, 69, 208}



Compound Data

Molecular weight	185.565	H bond acceptors	4	Rule of 5 violations	0
Compound type	aldehyde	H bond donors	0	ACD/ALogP	2.5
Phase 25°C	solid	Rotatable bonds	2	Predicted density	1.485 g/cm ³
SMILES	<chem>O=Cc1cc(ccc1Cl)[N+](=O)[O-]</chem>				
InChIKey	VFVHWCKUHAEDMY-UHFFFAOYSA-N				

Abraham Solute Descriptors

log S _w	E	S	A	B	V
-3.100	1.221	1.359	-0.054	0.182	0.954

Solubility Data

Solvent	Concentration (M)		Solvent bp °C
	Measured	Predicted	
acetonitrile	2.31	2.23	63.5
chloroform	2.90	2.49	61.2
DMSO	2.93	3.12	189
THF	2.79	2.45	68.3
toluene	1.74	2.15	110.6
1-butanol	-	0.16	117.7
1-decanol	-	0.13	227.8
1-heptanol	-	0.17	176.9
1-hexanol	-	0.18	158.2
1-octanol	-	0.20	194.7
1-pentanol	-	0.14	138.5
1-propanol	-	0.16	95.8
1,2-dichloroethane	-	4.18	83.5
1,4-dioxane	-	2.80	102.9
2-butanol	-	0.18	96.6
2-methyl-1-propanol	-	0.14	105.0
2-methyl-2-propanol	-	0.16	84.6
2-pentanol	-	0.12	118.8
2-propanol	-	0.13	73.0
2,2,4-trimethylpentane	-	0.12	98.8
3-methyl-1-butanol	-	0.13	131.2
acetone	-	2.29	46.5
benzene	-	2.62	78.8
butanone	-	2.94	75.6
butyl acetate	-	1.35	126.6
carbon disulfide	-	2.18	46.2
carbon tetrachloride	-	0.85	76.0
cyclohexane	-	0.26	80.7
decane	-	0.11	174.9
dibutyl ether	-	0.45	142.1
dichloromethane	-	4.35	39.6
diethyl ether	-	0.72	33.2
DMF	-	2.33	153.0
ethanol	-	0.24	72.6
ethyl acetate	-	1.51	73.9
ethylene glycol	-	0.05	197.5
heptane	-	0.08	98.8
hexadecane	-	0.14	286.6
hexane	-	0.13	68.5
methanol	-	0.26	48.1
methyl acetate	-	2.21	44.0
methyl tert-butyl ether	-	0.76	55.2
methylcyclohexane	-	0.14	101.1

nonane	-	0.14	151.7
octane	-	0.18	126.4
undecane	-	0.13	196.3
water	-	0.00	100.0

2-chloro-5-nitrobenzoic acid C₇H₄ClNO₄ - 22 solvents⁹⁰⁵



Compound Data					
Molecular weight	201.564	H bond acceptors	5	Rule of 5 violations	0
Compound type	carboxylic acid	H bond donors	1	ACD/ALogP	2.02
Phase 25°C	solid	Rotatable bonds	2	Predicted density	1.602 g/cm ³
SMILES	O=C(O)c1cc(ccc1Cl)[N+](=O)[O-]				
InChIKey	QUEKGYQTRJVEQC-UHFFFAOYSA-N				

Abraham Solute Descriptors

log S _w	E	S	A	B	V
-2.940	1.220	1.109	0.773	0.178	0.967

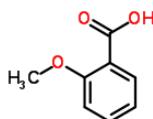
Solubility Data

Solvent	Concentration (M)		Solvent bp °C
	Measured	Predicted	
1-butanol	0.78	0.64	117.7
1-decanol	0.39	0.60	227.8
1-heptanol	0.54	0.63	176.9
1-hexanol	0.64	0.71	158.2
1-octanol	0.48	0.59	194.7
1-pentanol	0.74	0.76	138.5
1-propanol	0.95	1.09	95.8
2-butanol	0.91	0.67	96.6
2-methyl-1-propanol	0.63	0.62	105
2-methyl-2-propanol	1.21	0.82	84.6
2-pentanol	0.76	0.65	118.8
2-propanol	1.13	1.08	73
3-methyl-1-butanol	0.68	0.52	131.2
butyl acetate	0.46	0.59	126.6
dibutyl ether	0.10	0.08	142.1
diethyl ether	0.57	0.83	33.2
diisopropyl ether	0.19	*	68.3
ethanol	1.40	1.00	72.6
ethyl acetate	0.75	0.88	73.9
methyl acetate	0.89	0.57	44
pentyl acetate	0.43	*	149.9
THF	2.97	3.38	68.3
1,2-dichloroethane	-	0.04	83.5
1,4-dioxane	-	1.74	102.9
2,2,4-trimethylpentane	-	0.00	98.8
acetone	-	1.31	46.5
acetonitrile	-	0.16	63.5
benzene	-	0.02	78.8
butanone	-	1.22	75.6
carbon disulfide	-	0.01	46.2
carbon tetrachloride	-	0.00	76.0
chloroform	-	0.01	61.2
cyclohexane	-	0.00	80.7
decane	-	0.00	174.9
dichloromethane	-	0.02	39.6
DMF	-	6.55	153.0
DMSO	-	> 9	189.0
ethylene glycol	-	0.44	197.5
heptane	-	0.00	98.8
hexadecane	-	0.00	286.6

hexane	-	0.00	68.5
methanol	-	0.74	48.1
methyl tert-butyl ether	-	0.27	55.2
methylcyclohexane	-	0.00	101.1
nonane	-	0.00	151.7
octane	-	0.00	126.4
toluene	-	0.02	110.6
undecane	-	0.00	196.3
water	-	0.00	100.0

* This solvent doesn't have recorded Abraham coefficients.

2-methoxybenzoic acid C₈H₈O₃ - 31 solvents^{905, 34, 907}



Compound Data

Molecular weight	152.147	H bond acceptors	3	Rule of 5 violations	0
Compound type	carboxylic acid	H bond donors	1	ACD/ALogP	1.5
Phase 25°C	solid	Rotatable bonds	2	Predicted density	1.207 g/cm ³
SMILES	O=C(O)c1ccccc1OC				
InChIKey	ILUJQPXNXACGAN-UHFFFAOYSA-N				

Abraham Solute Descriptors

log S _w	E	S	A	B	V
-1.523	0.850	1.328	0.422	0.477	0.970

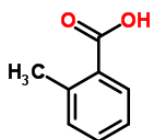
Solubility Data

Solvent	Concentration (M)		Solvent bp °C
	Measured	Predicted	
1-butanol	0.57	0.40	117.7
1-decanol	0.22	0.24	227.8
1-heptanol	0.34	0.33	176.9
1-hexanol	0.37	0.41	158.2
1-octanol	0.30	0.34	194.7
1-pentanol	0.47	0.39	138.5
1-propanol	0.76	0.57	95.8
1,4-dioxane	1.53	1.87	102.9
2-butanol	0.50	0.60	96.6
2-ethyl-1-hexanol	0.25	*	184.6
2-methyl-1-butanol	0.39	*	128.7
2-methyl-1-pentanol	0.35	*	148
2-methyl-1-propanol	0.41	0.48	105
2-methyl-2-propanol	0.53	0.59	84.6
2-pentanol	0.39	0.39	118.8
2-propanol	0.59	0.60	73
3-methyl-1-butanol	0.36	0.37	131.2
4-methyl-2-pentanol	0.32	*	133.5
butyl acetate	0.34	0.60	126.6
chloroform	0.46	0.31	61.2
dibutyl ether	0.04	0.08	142.1
diethyl ether	0.24	0.50	33.2
diisopropyl ether	0.06	*	68.3
ethanol	1.19	0.81	72.6
ethyl acetate	5.63	0.82	73.9
methanol	1.82	0.98	48.1
methyl acetate	0.86	1.19	44
pentyl acetate	0.26	*	149.9
propylene carbonate	0.99	*	332.3
THF	2.02	2.18	68.3
water	0.03	0.03	100
1,2-dichloroethane	-	0.36	83.5
2,2,4-trimethylpentane	-	0.00	98.8
acetone	-	1.56	46.5

acetonitrile	-	0.79	63.5
benzene	-	0.13	78.8
butanone	-	1.65	75.6
carbon disulfide	-	0.02	46.2
carbon tetrachloride	-	0.02	76.0
cyclohexane	-	0.00	80.7
decane	-	0.00	174.9
dichloromethane	-	0.39	39.6
DMF	-	5.74	153.0
DMSO	-	> 9	189.0
ethylene glycol	-	0.49	197.5
heptane	-	0.00	98.8
hexadecane	-	0.00	286.6
hexane	-	0.00	68.5
methyl tert-butyl ether	-	0.28	55.2
methylcyclohexane	-	0.00	101.1
nonane	-	0.00	151.7
octane	-	0.00	126.4
toluene	-	0.09	110.6
undecane	-	0.00	196.3

* This solvent doesn't have recorded Abraham coefficients.

2-methylbenzoic acid C₈H₈O₂ - 27 solvents^{905, 907}



Compound Data

Molecular weight	136.148	H bond acceptors	2	Rule of 5 violations	0
Compound type	carboxylic acid	H bond donors	1	ACD/ALogP	2.36
Phase 25°C	solid	Rotatable bonds	1	Predicted density	1.151 g/cm ³
SMILES	O=C(O)c1ccccc1C				
InChIKey	ZWLPBLYKEWSWPD-UHFFFAOYSA-N				

Abraham Solute Descriptors

log S _w	E	S	A	B	V
-2.000	0.854	0.689	0.368	0.284	0.857

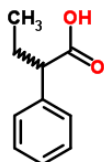
Solubility Data

Solvent	Concentration (M)		Solvent bp °C
	Measured	Predicted	
1-butanol	1.61	1.48	117.7
1-decanol	1.04	1.34	227.8
1-heptanol	1.28	1.39	176.9
1-hexanol	1.38	1.49	158.2
1-octanol	1.16	1.17	194.7
1-pentanol	1.49	1.61	138.5
1-propanol	1.77	1.82	95.8
1,4-dioxane	2.64	2.19	102.9
2-butanol	1.75	1.48	96.6
2-methyl-1-butanol	1.25	*	128.7
2-methyl-1-propanol	1.28	1.41	105
2-methyl-2-propanol	2.19	1.51	84.6
2-pentanol	1.68	1.59	118.8
2-propanol	1.95	1.64	73
3-methyl-1-butanol	1.34	1.39	131.2
4-methyl-2-pentanol	1.39	*	133.5
butyl acetate	1.17	1.40	126.6
dibutyl ether	0.58	0.43	142.1
diethyl ether	1.65	1.73	33.2
diisopropyl ether	0.86	*	68.3
ethanol	2.08	1.98	72.6
ethyl acetate	1.49	1.75	73.9
methyl acetate	1.51	1.50	44

pentyl acetate	1.04	*	149.9
propylene carbonate	0.46	*	332.3
THF	2.92	3.79	68.3
water	0.01	0.01	100
1,2-dichloroethane	-	0.47	83.5
2,2,4-trimethylpentane	-	0.04	98.8
acetone	-	2.00	46.5
acetonitrile	-	0.58	63.5
benzene	-	0.37	78.8
butanone	-	2.01	75.6
carbon disulfide	-	0.17	46.2
carbon tetrachloride	-	0.16	76.0
chloroform	-	0.43	61.2
cyclohexane	-	0.07	80.7
decane	-	0.05	174.9
dichloromethane	-	0.50	39.6
DMF	-	3.00	153.0
DMSO	-	4.83	189.0
ethylene glycol	-	0.58	197.5
heptane	-	0.06	98.8
hexadecane	-	0.04	286.6
hexane	-	0.05	68.5
methanol	-	1.58	48.1
methyl tert-butyl ether	-	1.03	55.2
methylcyclohexane	-	0.08	101.1
nonane	-	0.05	151.7
octane	-	0.06	126.4
toluene	-	0.33	110.6
undecane	-	0.05	196.3

* This solvent doesn't have recorded Abraham coefficients.

2-phenylbutyric acid C₁₀H₁₂O₂ - 5 solvents^{79, 83}



Compound Data			
Molecular weight	164.201	H bond acceptors	2
Compound type	carboxylic acid	H bond donors	1
Phase 25°C	solid	Rotatable bonds	3
SMILES	O=C(O)C(c1ccccc1)CC		
InChIKey	OFJWFSNDPCAWDK-UHFFFAOYSA-N		
Rule of 5 violations	0	ACD/ALogP	2.38
Predicted density	1.09 g/cm ³		

Abraham Solute Descriptors

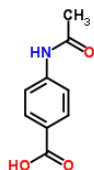
log S _w	E	S	A	B	V
-2.070	0.878	1.077	0.009	0.583	1.332

Solubility Data

Concentration (M)			
Solvent	Measured	Predicted	Solvent bp °C
acetonitrile	6.18	4.67	63.5
DMSO	5.97	5.21	189
ethanol	6.20	3.75	72.6
THF	5.96	12.21	68.3
toluene	5.35	9.46	110.6
1-butanol	-	2.55	117.7
1-decanol	-	2.06	227.8
1-heptanol	-	2.75	176.9
1-hexanol	-	2.76	158.2
1-octanol	-	2.24	194.7
1-pentanol	-	2.53	138.5
1-propanol	-	2.45	95.8
1,2-dichloroethane	-	> 9	83.5
1,4-dioxane	-	> 9	102.9

2-butanol	-	2.69	96.6
2-methyl-1-propanol	-	2.48	105.0
2-methyl-2-propanol	-	2.46	84.6
2-pentanol	-	2.67	118.8
2-propanol	-	2.09	73.0
2,2,4-trimethylpentane	-	0.76	98.8
3-methyl-1-butanol	-	2.76	131.2
acetone	-	7.27	46.5
benzene	-	> 9	78.8
butanone	-	> 9	75.6
butyl acetate	-	5.59	126.6
carbon disulfide	-	4.96	46.2
carbon tetrachloride	-	6.06	76.0
chloroform	-	> 9	61.2
cyclohexane	-	1.45	80.7
decane	-	0.71	174.9
dibutyl ether	-	1.81	142.1
dichloromethane	-	> 9	39.6
diethyl ether	-	3.94	33.2
DMF	-	> 9	153.0
ethyl acetate	-	5.82	73.9
ethylene glycol	-	0.55	197.5
heptane	-	0.77	98.8
hexadecane	-	0.79	286.6
hexane	-	0.83	68.5
methanol	-	3.18	48.1
methyl acetate	-	> 9	44.0
methyl tert-butyl ether	-	4.19	55.2
methylcyclohexane	-	1.68	101.1
nonane	-	0.87	151.7
octane	-	0.97	126.4
undecane	-	0.74	196.3
water	-	0.01	100.0

4-acetamidobenzoic acid C₉H₉NO₃ - 5 solvents¹³⁷



Compound Data				
Molecular weight	179.173	H bond acceptors	4	Rule of 5 violations 0
Compound type	carboxylic acid	H bond donors	2	ACD/ALogP 1.31
Phase 25°C	solid	Rotatable bonds	2	Predicted density 1.326 g/cm ³
SMILES	O=C(Nc1ccc(cc1)C(=O)O)C			
InChIKey	QCXJEYYXVJICE-UHFFFAOYSA-N			

Abraham Solute Descriptors					
log S _w	E	S	A	B	V
-2.120	1.279	1.112	0.793	0.734	1.104

Solubility Data			
Concentration (M)			
Solvent	Measured	Predicted	Solvent bp °C
acetonitrile	0.01	0.01	63.5
benzene	0.00	0.00	78.8
ethanol	0.23	0.22	72.6
methanol	0.19	0.20	48.1
THF	0.17	0.17	68.3
1-butanol	-	0.11	117.7
1-decanol	-	0.09	227.8
1-heptanol	-	0.09	176.9
1-hexanol	-	0.10	158.2
1-octanol	-	0.07	194.7
1-pentanol	-	0.13	138.5
1-propanol	-	0.19	95.8

1,2-dichloroethane	-	0.00	83.5
1,4-dioxane	-	0.09	102.9
2-butanol	-	0.15	96.6
2-methyl-1-propanol	-	0.12	105.0
2-methyl-2-propanol	-	0.12	84.6
2-pentanol	-	0.14	118.8
2-propanol	-	0.19	73.0
2,2,4-trimethylpentane	-	0.00	98.8
3-methyl-1-butanol	-	0.10	131.2
acetone	-	0.07	46.5
butanone	-	0.06	75.6
butyl acetate	-	0.03	126.6
carbon disulfide	-	0.00	46.2
carbon tetrachloride	-	0.00	76.0
chloroform	-	0.00	61.2
cyclohexane	-	0.00	80.7
decane	-	0.00	174.9
dibutyl ether	-	0.00	142.1
dichloromethane	-	0.00	39.6
diethyl ether	-	0.04	33.2
DMF	-	0.35	153.0
DMSO	-	2.29	189.0
ethyl acetate	-	0.04	73.9
ethylene glycol	-	0.35	197.5
heptane	-	0.00	98.8
hexadecane	-	0.00	286.6
hexane	-	0.00	68.5
methyl acetate	-	0.04	44.0
methyl tert-butyl ether	-	0.01	55.2
methylcyclohexane	-	0.00	101.1
nonane	-	0.00	151.7
octane	-	0.00	126.4
toluene	-	0.00	110.6
undecane	-	0.00	196.3
water	-	0.01	100.0

4-chloro-3-nitrobenzoic acid C₇H₄ClNO₄ - 30 solvents^{905, 907}



Compound Data			
Molecular weight	201.564	H bond acceptors	5
Compound type	carboxylic acid	H bond donors	1
Phase 25°C	solid	Rotatable bonds	2
SMILES	O=[N+](O-)[c1cc(ccc1Cl)C(=O)O]		
InChIKey	DFXQXFGFOLXAPO-UHFFFAOYSA-N		

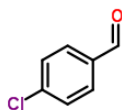
Abraham Solute Descriptors					
log S _w	E	S	A	B	V
-2.310	1.220	1.317	0.583	0.371	0.967

Solubility Data			
Concentration (M)			
Solvent	Measured	Predicted	Solvent bp °C
1-butanol	0.31	0.26	117.7
1-decanol	0.19	0.20	227.8
1-heptanol	0.25	0.23	176.9
1-hexanol	0.27	0.28	158.2
1-octanol	0.23	0.24	194.7
1-pentanol	0.27	0.28	138.5
1-propanol	0.37	0.41	95.8
1,4-dioxane	1.43	1.07	102.9
2-butanol	0.32	0.34	96.6

2-ethyl-1-hexanol	0.15	*	184.6
2-methyl-1-pentanol	0.19	*	148
2-methyl-1-propanol	0.19	0.27	105
2-methyl-2-propanol	0.38	0.33	84.6
2-pentanol	0.30	0.25	118.8
2-propanol	0.39	0.40	73
3-methyl-1-butanol	0.24	0.22	131.2
4-methyl-2-pentanol	0.23	*	133.5
butyl acetate	0.23	0.32	126.6
dibutyl ether	0.05	0.04	142.1
diethyl ether	0.24	0.32	33.2
diisopropyl ether	0.10	*	68.3
ethanol	0.55	0.49	72.6
ethyl acetate	0.36	0.47	73.9
methyl acetate	0.44	0.47	44
methyl butyrate	0.21	*	104.2
pentyl acetate	0.16	*	149.9
propyl acetate	0.26	*	101.4
propylene carbonate	0.15	*	332.3
THF	1.95	1.48	68.3
water	0.00	0.00	100
1,2-dichloroethane	-	0.08	83.5
2,2,4-trimethylpentane	-	0.00	98.8
acetone	-	0.83	46.5
acetonitrile	-	0.22	63.5
benzene	-	0.03	78.8
butanone	-	0.81	75.6
carbon disulfide	-	0.01	46.2
carbon tetrachloride	-	0.00	76.0
chloroform	-	0.04	61.2
cyclohexane	-	0.00	80.7
decane	-	0.00	174.9
dichloromethane	-	0.06	39.6
DMF	-	3.24	153.0
DMSO	-	> 9	189.0
ethylene glycol	-	0.34	197.5
heptane	-	0.00	98.8
hexadecane	-	0.00	286.6
hexane	-	0.00	68.5
methanol	-	0.49	48.1
methyl tert-butyl ether	-	0.13	55.2
methylcyclohexane	-	0.00	101.1
nonane	-	0.00	151.7
octane	-	0.00	126.4
toluene	-	0.02	110.6
undecane	-	0.00	196.3

* This solvent doesn't have recorded Abraham coefficients.

4-chlorobenzaldehyde C₇H₅ClO - 5 solvents^{7, 209}



Compound Data

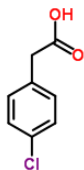
Molecular weight	140.567	H bond acceptors	1	Rule of 5 violations	0
Compound type	aldehyde	H bond donors	0	ACD/ALogP	2.21
Phase 25°C	solid	Rotatable bonds	1	Predicted density	1.243 g/cm ³
SMILES	<chem>O=Cc1ccc(Cl)cc1</chem>				
InChIKey	AVPYQKSLYISFPO-UHFFFAOYSA-N				

Abraham Solute Descriptors

log S _w	E	S	A	B	V
-2.270	0.933	0.716	0.080	0.087	0.781

Solubility Data			
Solvent	Concentration (M)		Solvent bp °C
	Measured	Predicted	
acetonitrile	5.58	3.70	63.5
chloroform	3.61	4.06	61.2
ethanol	2.81	2.50	72.6
methanol	3.55	2.05	48.1
THF	5.29	10.68	68.3
1-butanol	-	2.16	117.7
1-decanol	-	2.14	227.8
1-heptanol	-	2.24	176.9
1-hexanol	-	2.29	158.2
1-octanol	-	2.13	194.7
1-pentanol	-	2.15	138.5
1-propanol	-	2.20	95.8
1,2-dichloroethane	-	5.74	83.5
1,4-dioxane	-	7.75	102.9
2-butanol	-	1.92	96.6
2-methyl-1-propanol	-	1.80	105.0
2-methyl-2-propanol	-	1.92	84.6
2-pentanol	-	1.94	118.8
2-propanol	-	1.75	73.0
2,2,4-trimethylpentane	-	1.13	98.8
3-methyl-1-butanol	-	1.87	131.2
acetone	-	7.31	46.5
benzene	-	5.60	78.8
butanone	-	8.19	75.6
butyl acetate	-	6.21	126.6
carbon disulfide	-	6.18	46.2
carbon tetrachloride	-	3.23	76.0
cyclohexane	-	1.84	80.7
decane	-	1.14	174.9
dibutyl ether	-	3.34	142.1
dichloromethane	-	6.12	39.6
diethyl ether	-	5.72	33.2
DMF	-	5.32	153.0
DMSO	-	5.47	189.0
ethyl acetate	-	6.94	73.9
ethylene glycol	-	0.39	197.5
heptane	-	1.19	98.8
hexadecane	-	1.08	286.6
hexane	-	1.22	68.5
methyl acetate	-	6.42	44.0
methyl tert-butyl ether	-	5.11	55.2
methylcyclohexane	-	1.47	101.1
nonane	-	1.29	151.7
octane	-	1.54	126.4
toluene	-	5.48	110.6
undecane	-	1.12	196.3
water	-	0.01	100.0

4-chlorophenylacetic acid C₈H₇ClO₂ - 5 solvents^{4, 75, 73}



Compound Data			
Molecular weight	170.593	H bond acceptors	2
Compound type	carboxylic acid	H bond donors	1
Phase 25°C	solid	Rotatable bonds	2
SMILES	Clc1ccc(cc1)CC(=O)O		
InChIKey	CDPKJZJVTHSESZ-UHFFFAOYSA-N		
Rule of 5 violations	0	ACD/ALogP	2.1
Predicted density	1.324 g/cm ³		

Abraham Solute Descriptors

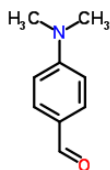
log S E S A B V

w					
-2.450	0.980	0.565	0.265	0.257	1.013

Solubility Data

Solvent	Concentration (M)		Solvent bp °C
	Measured	Predicted	
acetonitrile	1.67	1.22	63.5
DMSO	5.74	4.95	189
methanol	7.76	3.16	48.1
THF	4.45	11.84	68.3
toluene	0.89	2.33	110.6
1-butanol	-	4.56	117.7
1-decanol	-	5.30	227.8
1-heptanol	-	5.09	176.9
1-hexanol	-	4.85	158.2
1-octanol	-	3.82	194.7
1-pentanol	-	5.27	138.5
1-propanol	-	4.95	95.8
1,2-dichloroethane	-	2.16	83.5
1,4-dioxane	-	6.05	102.9
2-butanol	-	3.68	96.6
2-methyl-1-propanol	-	3.81	105.0
2-methyl-2-propanol	-	3.76	84.6
2-pentanol	-	5.07	118.8
2-propanol	-	4.04	73.0
2,2,4-trimethylpentane	-	0.48	98.8
3-methyl-1-butanol	-	4.39	131.2
acetone	-	5.13	46.5
benzene	-	2.38	78.8
butanone	-	5.65	75.6
butyl acetate	-	4.92	126.6
carbon disulfide	-	1.86	46.2
carbon tetrachloride	-	1.44	76.0
chloroform	-	2.18	61.2
cyclohexane	-	0.81	80.7
decane	-	0.53	174.9
dibutyl ether	-	2.25	142.1
dichloromethane	-	2.40	39.6
diethyl ether	-	6.20	33.2
DMF	-	5.89	153.0
ethyl acetate	-	5.56	73.9
ethylene glycol	-	0.78	197.5
heptane	-	0.74	98.8
hexadecane	-	0.46	286.6
hexane	-	0.53	68.5
methyl acetate	-	4.17	44.0
methyl tert-butyl ether	-	4.24	55.2
methylcyclohexane	-	0.98	101.1
nonane	-	0.58	151.7
octane	-	0.68	126.4
undecane	-	0.52	196.3
water	-	0.00	100.0

4-dimethylaminobenzaldehyde C₉H₁₁NO - 6 solvents^{208, 205}



Compound Data

Molecular weight	149.19	H bond acceptors	2	Rule of 5 violations	0
Compound type	aldehyde	H bond donors	0	ACD/ALogP	1.81
Phase 25°C	solid	Rotatable bonds	2	Predicted density	1.072 g/cm ³
SMILES	<chem>O=Cc1ccc(N(C)C)cc1</chem>				
InChIKey	BGNGWHSBYQYVRX-UHFFFAOYSA-N				

Abraham Solute Descriptors

$\log S_w$	E	S	A	B	V
-1.050	1.190	1.602	0.079	0.756	1.162

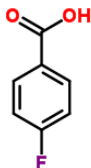
Solubility Data

Solvent	Concentration (M)		Solvent bp °C
	Measured	Predicted	
acetonitrile	2.60	2.77	63.5
chloroform	4.02	6.68	61.2
ethanol	0.63	0.86	72.6
methanol	1.36	1.22	48.1
THF	2.50	2.46	68.3
toluene	1.54	0.92	110.6
1-butanol	-	0.37	117.7
1-decanol	-	0.24	227.8
1-heptanol	-	0.31	176.9
1-hexanol	-	0.38	158.2
1-octanol	-	0.33	194.7
1-pentanol	-	0.34	138.5
1-propanol	-	0.43	95.8
1,2-dichloroethane	-	4.57	83.5
1,4-dioxane	-	3.07	102.9
2-butanol	-	0.63	96.6
2-methyl-1-propanol	-	0.42	105.0
2-methyl-2-propanol	-	0.40	84.6
2-pentanol	-	0.35	118.8
2-propanol	-	0.39	73.0
2,2,4-trimethylpentane	-	0.02	98.8
3-methyl-1-butanol	-	0.36	131.2
acetone	-	2.40	46.5
benzene	-	1.54	78.8
butanone	-	2.89	75.6
butyl acetate	-	0.92	126.6
carbon disulfide	-	0.22	46.2
carbon tetrachloride	-	0.34	76.0
cyclohexane	-	0.04	80.7
decane	-	0.02	174.9
dibutyl ether	-	0.12	142.1
dichloromethane	-	6.04	39.6
diethyl ether	-	0.49	33.2
DMF	-	4.88	153.0
DMSO	-	> 9	189.0
ethyl acetate	-	1.15	73.9
ethylene glycol	-	0.64	197.5
heptane	-	0.02	98.8
hexadecane	-	0.03	286.6
hexane	-	0.03	68.5
methyl acetate	-	2.74	44.0
methyl tert-butyl ether	-	0.41	55.2
methylcyclohexane	-	0.05	101.1
nonane	-	0.02	151.7
octane	-	0.03	126.4
undecane	-	0.02	196.3
water	-	0.09	100.0

4-fluorobenzoic acid $C_7H_5FO_2$ - 7 solvents^{106, 121, 907}

Compound Data

Molecular weight	140.112	H bond acceptors	2	Rule of 5 violations	0
Compound type	carboxylic acid	H bond donors	1	ACD/ALogP	2.07
Phase 25°C	solid	Rotatable bonds	1	Predicted density	1.319 g/cm ³



SMILES

O=C(O)c1ccc(F)cc1

InChIKey

BBYDXOIZLAWGSL-UHFFFAOYSA-N

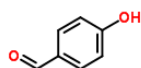
Abraham Solute Descriptors

log S _w	E	S	A	B	V
-2.000	0.726	0.720	0.400	0.168	0.680

Solubility Data

Solvent	Concentration (M)		Solvent bp °C
	Measured	Predicted	
acetonitrile	0.39	0.42	63.5
DMSO	4.19	4.36	189
ethanol	0.80	0.89	72.6
methanol	0.76	0.82	48.1
THF	2.49	1.98	68.3
toluene	0.00	0.12	110.6
water	0.01	0.01	100
1-butanol	-	0.64	117.7
1-decanol	-	0.50	227.8
1-heptanol	-	0.55	176.9
1-hexanol	-	0.63	158.2
1-octanol	-	0.52	194.7
1-pentanol	-	0.65	138.5
1-propanol	-	0.83	95.8
1,2-dichloroethane	-	0.20	83.5
1,4-dioxane	-	1.25	102.9
2-butanol	-	0.69	96.6
2-methyl-1-propanol	-	0.64	105.0
2-methyl-2-propanol	-	0.76	84.6
2-pentanol	-	0.63	118.8
2-propanol	-	0.79	73.0
2,2,4-trimethylpentane	-	0.02	98.8
3-methyl-1-butanol	-	0.57	131.2
acetone	-	1.24	46.5
benzene	-	0.13	78.8
butanone	-	1.18	75.6
butyl acetate	-	0.75	126.6
carbon disulfide	-	0.06	46.2
carbon tetrachloride	-	0.05	76.0
chloroform	-	0.14	61.2
cyclohexane	-	0.02	80.7
decane	-	0.02	174.9
dibutyl ether	-	0.22	142.1
dichloromethane	-	0.19	39.6
diethyl ether	-	0.91	33.2
DMF	-	1.89	153.0
ethyl acetate	-	0.99	73.9
ethylene glycol	-	0.30	197.5
heptane	-	0.02	98.8
hexadecane	-	0.01	286.6
hexane	-	0.02	68.5
methyl acetate	-	0.86	44.0
methyl tert-butyl ether	-	0.53	55.2
methylcyclohexane	-	0.02	101.1
nonane	-	0.02	151.7
octane	-	0.02	126.4
undecane	-	0.02	196.3

4-hydroxybenzaldehyde C₇H₆O₂ - 7 solvents^{208, 57, 205, 58, 88, 85, 909}



Compound Data

Molecular weight	122.121	H bond acceptors	2	Rule of 5 violations	0
Compound type	aldehyde	H bond donors	1	ACD/ALogP	1.39
Phase 25°C	solid	Rotatable bonds	2	Predicted density	1.226 g/cm ³
SMILES	<chem>O=Cc1ccc(O)cc1</chem>				
InChIKey	RGHHSNMVTDWUBI-UHFFFAOYSA-N				

Abraham Solute Descriptors

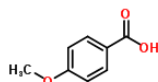
log S _w	E	S	A	B	V
-0.959	0.918	1.003	0.439	0.225	0.583

Solubility Data

Solvent	Concentration (M)		Solvent bp °C
	Measured	Predicted	
acetonitrile	1.46	1.38	63.5
chloroform	1.75	0.22	61.2
ethanol	2.52	1.65	72.6
methanol	3.39	1.97	48.1
THF	3.70	3.79	68.3
toluene	0.02	0.16	110.6
water	0.11	0.11	100
1-butanol	-	0.96	117.7
1-decanol	-	0.67	227.8
1-heptanol	-	0.73	176.9
1-hexanol	-	0.92	158.2
1-octanol	-	0.81	194.7
1-pentanol	-	0.93	138.5
1-propanol	-	1.38	95.8
1,2-dichloroethane	-	0.40	83.5
1,4-dioxane	-	3.04	102.9
2-butanol	-	1.29	96.6
2-methyl-1-propanol	-	1.01	105.0
2-methyl-2-propanol	-	1.19	84.6
2-pentanol	-	0.87	118.8
2-propanol	-	1.32	73.0
2,2,4-trimethylpentane	-	0.01	98.8
3-methyl-1-butanol	-	0.79	131.2
acetone	-	3.05	46.5
benzene	-	0.19	78.8
butanone	-	2.72	75.6
butyl acetate	-	1.30	126.6
carbon disulfide	-	0.06	46.2
carbon tetrachloride	-	0.05	76.0
cyclohexane	-	0.01	80.7
decane	-	0.01	174.9
dibutyl ether	-	0.24	142.1
dichloromethane	-	0.34	39.6
diethyl ether	-	1.34	33.2
DMF	-	5.10	153.0
DMSO	-	> 9	189.0
ethyl acetate	-	1.87	73.9
ethylene glycol	-	1.26	197.5
heptane	-	0.01	98.8
hexadecane	-	0.01	286.6
hexane	-	0.01	68.5
methyl acetate	-	1.96	44.0
methyl tert-butyl ether	-	0.69	55.2
methylcyclohexane	-	0.01	101.1
nonane	-	0.01	151.7

octane	-	0.02	126.4
undecane	-	0.01	196.3

4-methoxybenzoic acid C₈H₈O₃ - 22 solvents⁹⁰⁵



Compound Data			
Molecular weight	152.147	H bond acceptors	3
Compound type	carboxylic acid	H bond donors	1
Phase 25°C	solid	Rotatable bonds	2
SMILES	COc1ccc(cc1)C(O)=O		
InChIKey	ZEYHEAKUIGZSGI-UHFFFAOYSA-N		
		Rule of 5 violations	0
		ACD/ALogP	1.96
		Predicted density	1.207 g/cm ³

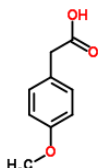
Abraham Solute Descriptors					
log S _w	E	S	A	B	V
-1.880	0.850	1.290	0.404	0.552	0.970

Solubility Data			
Concentration (M)			
Solvent	Measured	Predicted	Solvent bp °C
1-butanol	0.12	0.10	117.7
1-decanol	0.07	0.06	227.8
1-heptanol	0.09	0.08	176.9
1-hexanol	0.10	0.10	158.2
1-octanol	0.08	0.08	194.7
1-pentanol	0.10	0.10	138.5
1-propanol	0.13	0.14	95.8
1,4-dioxane	0.39	0.37	102.9
2-butanol	0.13	0.15	96.6
2-ethyl-1-hexanol	0.07	*	184.6
2-methyl-1-propanol	0.08	0.12	105
2-methyl-2-propanol	0.17	0.14	84.6
2-propanol	0.14	0.14	73
3-methyl-1-butanol	0.08	0.10	131.2
butyl acetate	0.08	0.12	126.6
dibutyl ether	0.02	0.02	142.1
diethyl ether	0.09	0.10	33.2
diisopropyl ether	0.03	*	68.3
ethanol	0.20	0.21	72.6
ethyl acetate	0.13	0.17	73.9
pentyl acetate	0.06	*	149.9
THF	0.70	0.43	68.3
1,2-dichloroethane	-	0.09	83.5
2-pentanol	-	0.10	118.8
2,2,4-trimethylpentane	-	0.00	98.8
acetone	-	0.32	46.5
acetonitrile	-	0.17	63.5
benzene	-	0.03	78.8
butanone	-	0.33	75.6
carbon disulfide	-	0.00	46.2
carbon tetrachloride	-	0.01	76.0
chloroform	-	0.09	61.2
cyclohexane	-	0.00	80.7
decane	-	0.00	174.9
dichloromethane	-	0.10	39.6
DMF	-	1.05	153.0
DMSO	-	3.09	189.0
ethylene glycol	-	0.15	197.5
heptane	-	0.00	98.8
hexadecane	-	0.00	286.6
hexane	-	0.00	68.5
methanol	-	0.26	48.1
methyl acetate	-	0.25	44.0

methyl tert-butyl ether	-	0.06	55.2
methylcyclohexane	-	0.00	101.1
nonane	-	0.00	151.7
octane	-	0.00	126.4
toluene	-	0.02	110.6
undecane	-	0.00	196.3
water	-	0.01	100.0

* This solvent doesn't have recorded Abraham coefficients.

4-methoxyphenylacetic acid C₉H₁₀O₃ - 6 solvents^{89, 136, 92, 910}



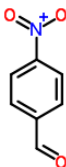
Compound Data			
Molecular weight	166.174	H bond acceptors	3
Compound type	carboxylic acid	H bond donors	1
Phase 25°C	solid	Rotatable bonds	3
SMILES	O=C(O)Cc1ccc(OC)cc1		
InChIKey	NRPFNQUDKRYCNX-UHFFFAOYSA-N		
Rule of 5 violations	0		
ACD/ALogP	1.42		
Predicted density	1.179 g/cm ³		

Abraham Solute Descriptors					
log S _w	E	S	A	B	V
-1.398	0.877	1.137	0.101	0.678	1.189

Solubility Data			
Concentration (M)			
Solvent	Measured	Predicted	Solvent bp °C
acetonitrile	2.23	2.08	63.5
DMSO	4.50	4.37	189
methanol	2.50	2.07	48.1
THF	3.31	4.06	68.3
toluene	0.37	1.66	110.6
water	0.04	0.04	100
1-butanol	-	1.13	117.7
1-decanol	-	0.80	227.8
1-heptanol	-	1.03	176.9
1-hexanol	-	1.14	158.2
1-octanol	-	0.90	194.7
1-pentanol	-	1.10	138.5
1-propanol	-	1.21	95.8
1,2-dichloroethane	-	4.67	83.5
1,4-dioxane	-	3.51	102.9
2-butanol	-	1.47	96.6
2-methyl-1-propanol	-	1.21	105.0
2-methyl-2-propanol	-	1.16	84.6
2-pentanol	-	1.20	118.8
2-propanol	-	1.09	73.0
2,2,4-trimethylpentane	-	0.10	98.8
3-methyl-1-butanol	-	1.21	131.2
acetone	-	2.85	46.5
benzene	-	2.42	78.8
butanone	-	3.51	75.6
butyl acetate	-	1.68	126.6
carbon disulfide	-	0.53	46.2
carbon tetrachloride	-	0.91	76.0
chloroform	-	> 9	61.2
cyclohexane	-	0.18	80.7
decane	-	0.09	174.9
dibutyl ether	-	0.38	142.1
dichloromethane	-	7.21	39.6
diethyl ether	-	1.22	33.2
DMF	-	5.11	153.0
ethyl acetate	-	1.93	73.9

ethylene glycol	-	0.67	197.5
heptane	-	0.11	98.8
hexadecane	-	0.11	286.6
hexane	-	0.12	68.5
methyl acetate	-	3.37	44.0
methyl tert-butyl ether	-	1.09	55.2
methylcyclohexane	-	0.25	101.1
nonane	-	0.12	151.7
octane	-	0.13	126.4
undecane	-	0.09	196.3

4-nitrobenzaldehyde C₇H₅NO₃ - 10 solvents^{111, 98, 904, 212, 82, 122}



Compound Data

Molecular weight	151.12	H bond acceptors	4	Rule of 5 violations	0
Compound type	aldehyde	H bond donors	0	ACD/ALogP	1.56
Phase 25°C	solid	Rotatable bonds	2	Predicted density	1.338 g/cm ³
SMILES	<chem>c1cc(C=O)ccc1[N+](=O)[O-]</chem>				
InChIKey	BXRFSNOROTLV-UHFFFAOYSA-N				

Abraham Solute Descriptors

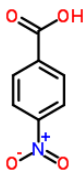
log S _w	E	S	A	B	V
-2.280	1.049	1.634	-0.031	0.289	0.780

Solubility Data

Solvent	Concentration (M)		Solvent bp °C
	Measured	Predicted	
acetonitrile	1.13	1.41	63.5
benzene	0.46	0.44	78.8
carbon tetrachloride	0.07	0.09	76
chloroform	1.02	0.74	61.2
cyclohexane	0.01	0.02	80.7
dichloromethane	1.29	1.33	39.6
DMF	1.68	0.99	153
DMSO	1.24	2.70	189
THF	0.88	0.53	68.3
toluene	0.46	0.30	110.6
1-butanol	-	0.03	117.7
1-decanol	-	0.02	227.8
1-heptanol	-	0.02	176.9
1-hexanol	-	0.03	158.2
1-octanol	-	0.04	194.7
1-pentanol	-	0.02	138.5
1-propanol	-	0.03	95.8
1,2-dichloroethane	-	1.25	83.5
1,4-dioxane	-	0.84	102.9
2-butanol	-	0.05	96.6
2-methyl-1-propanol	-	0.03	105.0
2-methyl-2-propanol	-	0.04	84.6
2-pentanol	-	0.02	118.8
2-propanol	-	0.03	73.0
2,2,4-trimethylpentane	-	0.01	98.8
3-methyl-1-butanol	-	0.02	131.2
acetone	-	0.76	46.5
butanone	-	0.91	75.6
butyl acetate	-	0.28	126.6
carbon disulfide	-	0.16	46.2
decane	-	0.01	174.9
dibutyl ether	-	0.06	142.1
diethyl ether	-	0.12	33.2
ethanol	-	0.06	72.6
ethyl acetate	-	0.35	73.9

ethylene glycol	-	0.03	197.5
heptane	-	0.00	98.8
hexadecane	-	0.01	286.6
methanol	-	0.11	48.1
methyl acetate	-	0.76	44.0
methyl tert-butyl ether	-	0.13	55.2
methylcyclohexane	-	0.01	101.1
nonane	-	0.01	151.7
octane	-	0.01	126.4
undecane	-	0.01	196.3
water	-	0.01	100.0

4-nitrobenzoic acid C₇H₅NO₄ - 29 solvents⁹⁰⁵



Compound Data

Molecular weight	167.119	H bond acceptors	5	Rule of 5 violations	0
Compound type	carboxylic acid	H bond donors	1	ACD/ALogP	1.89
Phase 25°C	solid	Rotatable bonds	2	Predicted density	1.468 g/cm ³
SMILES	O=[N+](O-)[C-]1ccc(C(=O)O)cc1				
InChIKey	OTLNPYWUJOZPPA-UHFFFAOYSA-N				

Abraham Solute Descriptors

log S _w	E	S	A	B	V
-2.120	1.048	1.301	0.518	0.349	0.793

Solubility Data

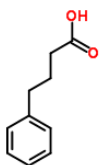
Concentration (M)

Solvent	Measured	Predicted	Solvent bp °C
1-butanol	0.09	0.08	117.7
1-decanol	0.05	0.05	227.8
1-heptanol	0.08	0.06	176.9
1-hexanol	0.08	0.08	158.2
1-octanol	0.06	0.07	194.7
1-pentanol	0.09	0.08	138.5
1-propanol	0.11	0.13	95.8
1,4-dioxane	0.47	0.38	102.9
2-butanol	0.10	0.12	96.6
2-methyl-1-butanol	0.05	*	128.7
2-methyl-1-pentanol	0.05	*	148
2-methyl-1-propanol	0.07	0.09	105
2-methyl-2-butanol	0.17	*	102
2-methyl-2-propanol	0.15	0.11	84.6
2-pentanol	0.08	0.07	118.8
2-propanol	0.11	0.13	73
3-methyl-1-butanol	0.07	0.07	131.2
4-methyl-2-pentanol	0.07	*	133.5
butyl acetate	0.08	0.12	126.6
dibutyl ether	0.02	0.01	142.1
diethyl ether	0.10	0.11	33.2
diisopropyl ether	0.03	*	68.3
ethanol	0.14	0.16	72.6
ethyl acetate	0.13	0.17	73.9
methanol	0.18	0.20	48.1
methyl acetate	0.14	0.20	44
pentyl acetate	0.05	*	149.9
propylene carbonate	0.06	*	332.3
THF	0.78	0.45	68.3
1,2-dichloroethane	-	0.04	83.5
2,2,4-trimethylpentane	-	0.00	98.8
acetone	-	0.33	46.5
acetonitrile	-	0.13	63.5

benzene	-	0.01	78.8
butanone	-	0.31	75.6
carbon disulfide	-	0.00	46.2
carbon tetrachloride	-	0.00	76.0
chloroform	-	0.02	61.2
cyclohexane	-	0.00	80.7
decane	-	0.00	174.9
dichloromethane	-	0.03	39.6
DMF	-	1.02	153.0
DMSO	-	6.21	189.0
ethylene glycol	-	0.14	197.5
heptane	-	0.00	98.8
hexadecane	-	0.00	286.6
hexane	-	0.00	68.5
methyl tert-butyl ether	-	0.05	55.2
methylcyclohexane	-	0.00	101.1
nonane	-	0.00	151.7
octane	-	0.00	126.4
toluene	-	0.01	110.6
undecane	-	0.00	196.3
water	-	0.01	100.0

* This solvent doesn't have recorded Abraham coefficients.

4-phenylbutyric acid C₁₀H₁₂O₂ - 5 solvents⁷²



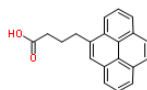
Compound Data			
Molecular weight	164.201	H bond acceptors	2
Compound type	carboxylic acid	H bond donors	1
Phase 25°C	solid	Rotatable bonds	4
SMILES	O=C(O)CCCC1CCCCC1		
InChIKey	OBKXEAXTFZPCHS-UHFFFAOYSA-N		
Rule of 5 violations	0	ACD/ALogP	2.42
Predicted density	1.095 g/cm ³		

Abraham Solute Descriptors					
log S _w	E	S	A	B	V
-2.510	0.896	3.980	0.540	-0.076	1.321

Solubility Data			
Concentration (M)			
Solvent	Measured	Predicted	Solvent bp °C
1-hexanol	0.19	0.21	158.2
chloroform	3.99	3.67	61.2
diethyl ether	4.02	5.98	33.2
methanol	4.54	2.27	48.1
toluene	4.06	0.97	110.6
1-butanol	-	0.14	117.7
1-decanol	-	0.02	227.8
1-heptanol	-	0.12	176.9
1-octanol	-	0.42	194.7
1-pentanol	-	0.07	138.5
1-propanol	-	0.31	95.8
1,2-dichloroethane	-	> 9	83.5
1,4-dioxane	-	> 9	102.9
2-butanol	-	0.42	96.6
2-methyl-1-propanol	-	0.25	105.0
2-methyl-2-propanol	-	1.18	84.6
2-pentanol	-	0.05	118.8
2-propanol	-	0.51	73.0
2,2,4-trimethylpentane	-	0.00	98.8
3-methyl-1-butanol	-	0.08	131.2
acetone	-	> 9	46.5
acetonitrile	-	> 9	63.5

benzene	-	2.33	78.8
butanone	-	> 9	75.6
butyl acetate	-	> 9	126.6
carbon disulfide	-	0.25	46.2
carbon tetrachloride	-	0.01	76.0
cyclohexane	-	0.00	80.7
decane	-	0.00	174.9
dibutyl ether	-	0.62	142.1
dichloromethane	-	> 9	39.6
DMF	-	> 9	153.0
DMSO	-	> 9	189.0
ethyl acetate	-	> 9	73.9
ethylene glycol	-	0.20	197.5
heptane	-	0.00	98.8
hexadecane	-	0.00	286.6
hexane	-	0.00	68.5
methyl acetate	-	> 9	44.0
methyl tert-butyl ether	-	3.92	55.2
methylcyclohexane	-	0.00	101.1
nonane	-	0.00	151.7
octane	-	0.00	126.4
THF	-	> 9	68.3
undecane	-	0.00	196.3
water	-	0.00	100.0

4-pyrenebutanoic acid C₂₀H₁₆O₂ - 16 solvents ^{61, 99, 51, 30, 24, 91, 84}



Compound Data					
Molecular weight	288.34	H bond acceptors	2	Rule of 5 violations	1
Compound type	carboxylic acid	H bond donors	1	ACD/ALogP	5.37
Phase 25°C	solid	Rotatable bonds	4	Predicted density	1.296 g/cm ³
SMILES	O=C(O)CCCc4cc2cccc1ccc3c(c12)c4ccc3				
InChIKey	GSBSDUZYVSCTUKA-UHFFFAOYSA-N				

Abraham Solute Descriptors

log S _w	E	S	A	B	V
-7.150	3.727	2.030	0.411	0.855	2.385

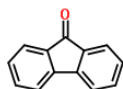
Solubility Data

Solvent	Concentration (M)		Solvent bp °C
	Measured	Predicted	
2-propanol	0.06	0.04	73.0
acetonitrile	0.00	0.01	63.5
benzene	0.00	0.11	78.8
carbon tetrachloride	0.00	0.02	76
chloroform	0.03	0.06	61.2
cyclohexane	0.00	0.00	80.7
cyclopentane	0.00	*	49.2
dichloromethane	0.07	0.05	39.6
diethyl ether	0.02	0.08	33.2
DMF	1.88	0.51	153
DMSO	2.07	1.36	189
ethanol	0.06	0.09	72.6
hexane	0.00	0.00	68.5
methanol	0.01	0.03	48.1
THF	0.55	0.87	68.3
toluene	0.00	0.09	110.6
1-butanol	-	0.06	117.7
1-decanol	-	0.27	227.8
1-heptanol	-	0.12	176.9
1-hexanol	-	0.10	158.2
1-octanol	-	0.09	194.7

1-pentanol	-	0.11	138.5
1-propanol	-	0.07	95.8
1,2-dichloroethane	-	0.10	83.5
1,4-dioxane	-	0.48	102.9
2-butanol	-	0.04	96.6
2-methyl-1-propanol	-	0.03	105.0
2-methyl-2-propanol	-	0.02	84.6
2-pentanol	-	0.07	118.8
2,2,4-trimethylpentane	-	0.00	98.8
3-methyl-1-butanol	-	0.05	131.2
acetone	-	0.15	46.5
butanone	-	0.21	75.6
butyl acetate	-	0.10	126.6
carbon disulfide	-	0.07	46.2
decane	-	0.00	174.9
dibutyl ether	-	0.01	142.1
ethyl acetate	-	0.12	73.9
ethylene glycol	-	0.03	197.5
heptane	-	0.00	98.8
hexadecane	-	0.00	286.6
methyl acetate	-	0.08	44.0
methyl tert-butyl ether	-	0.02	55.2
methylcyclohexane	-	0.00	101.1
nonane	-	0.00	151.7
octane	-	0.00	126.4
undecane	-	0.00	196.3
water	-	0.00	100.0

* This solvent doesn't have recorded Abraham coefficients.

9-fluorenone C₁₃H₈O - 43 solvents⁹⁰⁵



Compound Data			
Molecular weight	180.202	H bond acceptors	1
Compound type	non-Ugi related	H bond donors	0
Phase 25°C	solid	Rotatable bonds	0
SMILES	O=C3c1ccccc1c2c3ccc2		
InChIKey	YLQWCDOCJODRMT-UHFFFAOYSA-N		
Rule of 5 violations	0	ACD/ALogP	3.58
Predicted density	1.244 g/cm ³		

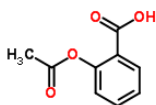
Abraham Solute Descriptors					
log S _w	E	S	A	B	V
-3.910	1.638	1.392	0.097	0.233	1.247

Solubility Data			
Concentration (M)			
Solvent	Measured	Predicted	Solvent bp °C
1-butanol	0.37	0.36	117.7
1-decanol	0.42	0.44	227.8
1-heptanol	0.43	0.46	176.9
1-hexanol	0.41	0.46	158.2
1-octanol	0.43	0.47	194.7
1-pentanol	0.41	0.38	138.5
1-propanol	0.38	0.39	95.8
2-butanol	0.33	0.34	96.6
2-ethyl-1-hexanol	0.35	*	184.6
2-methyl-1-pentanol	0.36	*	148
2-methyl-1-propanol	0.25	0.28	105
2-methyl-2-butanol	0.40	*	102
2-methyl-2-propanol	0.31	0.29	84.6
2-pentanol	0.35	0.31	118.8
2-propanol	0.29	0.29	73
2,2,4-trimethylpentane	0.07	0.08	98.8

3-methyl-1-butanol	0.31	0.29	131.2
4-methyl-2-pentanol	0.29	*	133.5
acetonitrile	1.57	1.27	63.5
benzene	2.61	2.55	78.8
butyronitrile	1.93	*	117.3
carbon tetrachloride	1.83	0.75	76
cyclohexane	0.15	0.25	80.7
cyclooctane	0.17	*	152
cyclopentanol	0.82	*	140.8
decane	0.12	0.10	174.9
dibutyl ether	0.37	0.61	142.1
dichloromethane	4.03	2.89	39.6
diethyl ether	0.88	1.36	33.2
diisopropyl ether	0.37	*	68.3
ethanol	3.08	0.50	72.6
heptane	0.11	0.08	98.8
hexadecane	0.12	0.12	286.6
hexane	0.10	0.09	68.5
methanol	0.37	0.37	48.1
methyl tert-butyl ether	0.76	1.06	55.2
methylcyclohexane	0.14	0.15	101.1
nonane	0.12	0.12	151.7
octane	0.11	0.16	126.4
propionitrile	1.99	*	91.3
tert-butylcyclohexane	0.12	*	168.3
toluene	2.17	2.23	110.6
undecane	0.12	0.12	196.3
1,2-dichloroethane	-	3.24	83.5
1,4-dioxane	-	4.70	102.9
acetone	-	3.14	46.5
butanone	-	4.10	75.6
butyl acetate	-	2.10	126.6
carbon disulfide	-	2.41	46.2
chloroform	-	1.79	61.2
DMF	-	4.62	153.0
DMSO	-	6.16	189.0
ethyl acetate	-	2.33	73.9
ethylene glycol	-	0.08	197.5
methyl acetate	-	2.50	44.0
THF	-	5.44	68.3
water	-	0.00	100.0

* This solvent doesn't have recorded Abraham coefficients.

acetylsalicylic acid C₉H₈O₄ - 6 solvents^{72, 34, 903, 907}



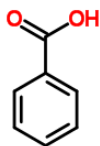
Compound Data			
Molecular weight	180.157	H bond acceptors	4
Compound type	carboxylic acid	H bond donors	1
Phase 25°C	solid	Rotatable bonds	3
SMILES	<chem>O=C(Oc1ccccc1C(=O)O)C</chem>		
InChIKey	BSYNRYMUTXBXSQ-UHFFFAOYSA-N		
Rule of 5 violations	0	ACD/ALogP	1.19
		Predicted density	1.29 g/cm ³

Abraham Solute Descriptors					
log S _w	E	S	A	B	V
-1.602	0.946	5.432	0.815	-0.028	1.170

Solubility Data			
Concentration (M)			
Solvent	Measured	Predicted	Solvent bp °C
1-hexanol	0.00	0.01	158.2
chloroform	0.18	0.16	61.2

diethyl ether	0.17	0.32	33.2
methanol	1.30	0.43	48.1
toluene	0.00	0.01	110.6
water	0.03	0.03	100
1-butanol	-	0.00	117.7
1-decanol	-	0.00	227.8
1-heptanol	-	0.00	176.9
1-octanol	-	0.02	194.7
1-pentanol	-	0.00	138.5
1-propanol	-	0.01	95.8
1,2-dichloroethane	-	7.20	83.5
1,4-dioxane	-	> 9	102.9
2-butanol	-	0.03	96.6
2-methyl-1-propanol	-	0.01	105.0
2-methyl-2-propanol	-	0.09	84.6
2-pentanol	-	0.00	118.8
2-propanol	-	0.03	73.0
2,2,4-trimethylpentane	-	0.00	98.8
3-methyl-1-butanol	-	0.00	131.2
acetone	-	> 9	46.5
acetonitrile	-	> 9	63.5
benzene	-	0.05	78.8
butanone	-	> 9	75.6
butyl acetate	-	5.04	126.6
carbon disulfide	-	0.00	46.2
carbon tetrachloride	-	0.00	76.0
cyclohexane	-	0.00	80.7
decane	-	0.00	174.9
dibutyl ether	-	0.01	142.1
dichloromethane	-	3.00	39.6
DMF	-	> 9	153.0
DMSO	-	> 9	189.0
ethyl acetate	-	> 9	73.9
ethylene glycol	-	0.09	197.5
heptane	-	0.00	98.8
hexadecane	-	0.00	286.6
hexane	-	0.00	68.5
methyl acetate	-	> 9	44.0
methyl tert-butyl ether	-	0.15	55.2
methylcyclohexane	-	0.00	101.1
nonane	-	0.00	151.7
octane	-	0.00	126.4
THF	-	> 9	68.3
undecane	-	0.00	196.3

benzoic acid C₇H₆O₂ - 10 solvents ^{155, 37, 902, 58, 160, 43, 136, 9, 907, 900}



Compound Data			
Molecular weight	122.121	H bond acceptors	2
Compound type	carboxylic acid	H bond donors	1
Phase 25°C	solid	Rotatable bonds	1
SMILES	O=C(O)c1ccccc1		
InChIKey	WPYMKLBDIGXBTP-UHFFFAOYSA-N		
Rule of 5 violations	0	ACD/ALogP	1.9
Predicted density	1.197 g/cm ³		

Abraham Solute Descriptors

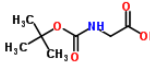
log S _w	E	S	A	B	V
-1.538	0.788	0.144	0.100	0.239	0.618

Solubility Data

Concentration (M)			
Solvent	Measured	Predicted	Solvent bp °C
1-octanol	1.48	1.81	194.7

acetone	1.35	1.75	46.5
acetonitrile	0.75	0.72	63.5
benzene	0.48	1.80	78.8
chloroform	1.80	1.75	61.2
ethanol	2.55	2.69	72.6
methanol	2.84	1.99	48.1
THF	3.37	2.83	68.3
toluene	0.65	1.87	110.6
water	0.03	0.03	100
1-butanol	-	2.58	117.7
1-decanol	-	2.99	227.8
1-heptanol	-	2.41	176.9
1-hexanol	-	2.38	158.2
1-pentanol	-	2.85	138.5
1-propanol	-	2.51	95.8
1,2-dichloroethane	-	1.37	83.5
1,4-dioxane	-	1.56	102.9
2-butanol	-	2.18	96.6
2-methyl-1-propanol	-	2.13	105.0
2-methyl-2-propanol	-	1.76	84.6
2-pentanol	-	2.93	118.8
2-propanol	-	1.92	73.0
2,2,4-trimethylpentane	-	1.47	98.8
3-methyl-1-butanol	-	2.53	131.2
butanone	-	1.68	75.6
butyl acetate	-	1.95	126.6
carbon disulfide	-	1.61	46.2
carbon tetrachloride	-	2.03	76.0
cyclohexane	-	1.89	80.7
decane	-	1.29	174.9
dibutyl ether	-	1.45	142.1
dichloromethane	-	1.68	39.6
diethyl ether	-	2.70	33.2
DMF	-	0.64	153.0
DMSO	-	0.57	189.0
ethyl acetate	-	2.19	73.9
ethylene glycol	-	0.66	197.5
heptane	-	2.32	98.8
hexadecane	-	1.15	286.6
hexane	-	1.66	68.5
methyl acetate	-	1.73	44.0
methyl tert-butyl ether	-	2.23	55.2
methylcyclohexane	-	2.89	101.1
nonane	-	1.53	151.7
octane	-	1.56	126.4
undecane	-	1.11	196.3

boc-glycine C₇H₁₃NO₄ - 12 solvents ^{143, 71, 207, 135, 133, 116}

Compound Data						
	Molecular weight	175.182	H bond acceptors	5	Rule of 5 violations	0
	Compound type	carboxylic acid	H bond donors	2	ACD/ALogP	0.75
	Phase 25°C	solid	Rotatable bonds	4	Predicted density	1.159 g/cm³
	SMILES	O=C(OC(C)(C)C)NCC(=O)O				
	InChIKey	VRPJIFMKZZEXLR-UHFFFAOYSA-N				

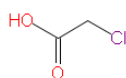
Abraham Solute Descriptors

log S _w	E	S	A	B	V
-1.260	0.402	0.823	0.255	0.784	1.338

Solubility Data

Solvent	Concentration (M)		Solvent bp °C
	Measured	Predicted	
2-propanol	3.63	4.15	73.0
acetonitrile	2.46	1.29	63.5
benzene	0.25	1.59	78.8
chloroform	3.85	9.41	61.2
dichloromethane	4.14	5.56	39.6
diethyl ether	2.65	2.18	33.2
DMSO	4.78	3.87	189
ethanol	4.11	5.88	72.6
hexane	0.25	0.12	68.5
methanol	4.72	5.01	48.1
THF	3.72	6.26	68.3
toluene	0.19	1.08	110.6
1-butanol	-	3.70	117.7
1-decanol	-	2.30	227.8
1-heptanol	-	3.43	176.9
1-hexanol	-	3.55	158.2
1-octanol	-	2.30	194.7
1-pentanol	-	3.85	138.5
1-propanol	-	4.06	95.8
1,2-dichloroethane	-	2.79	83.5
1,4-dioxane	-	3.70	102.9
2-butanol	-	4.29	96.6
2-methyl-1-propanol	-	4.37	105.0
2-methyl-2-propanol	-	4.59	84.6
2-pentanol	-	4.80	118.8
2,2,4-trimethylpentane	-	0.10	98.8
3-methyl-1-butanol	-	4.73	131.2
acetone	-	2.97	46.5
butanone	-	3.73	75.6
butyl acetate	-	2.13	126.6
carbon disulfide	-	0.25	46.2
carbon tetrachloride	-	0.73	76.0
cyclohexane	-	0.14	80.7
decane	-	0.10	174.9
dibutyl ether	-	0.51	142.1
DMF	-	> 9	153.0
ethyl acetate	-	2.40	73.9
ethylene glycol	-	1.27	197.5
heptane	-	0.14	98.8
hexadecane	-	0.09	286.6
methyl acetate	-	3.62	44.0
methyl tert-butyl ether	-	1.80	55.2
methylcyclohexane	-	0.29	101.1
nonane	-	0.11	151.7
octane	-	0.12	126.4
undecane	-	0.09	196.3
water	-	0.05	100.0

chloroacetic acid C₂H₃ClO₂ - 5 solvents⁹⁵



Compound Data				
Molecular weight	94.497	H bond acceptors	2	Rule of 5 violations 0
Compound type	carboxylic acid	H bond donors	1	ACD/ALogP 0.18
Phase 25°C	solid	Rotatable bonds	1	Predicted density 1.398 g/cm ³
SMILES	CIC(=O)O			
InChIKey	FOCAUTSVDIKZOP-UHFFFAOYSA-N			

Abraham Solute Descriptors

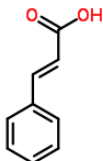
log S _w	E	S	A	B	V
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0.470 0.502 0.372 0.096 0.042 0.114

Solubility Data

Solvent	Concentration (M)		Solvent bp °C
	Measured	Predicted	
acetonitrile	12.45	12.35	63.5
DMSO	11.20	11.16	189
methanol	9.45	9.23	48.1
THF	9.63	9.88	68.3
toluene	1.41	4.33	110.6
1-butanol	-	5.23	117.7
1-decanol	-	3.70	227.8
1-heptanol	-	3.58	176.9
1-hexanol	-	4.39	158.2
1-octanol	-	3.92	194.7
1-pentanol	-	4.63	138.5
1-propanol	-	5.78	95.8
1,2-dichloroethane	-	6.00	83.5
1,4-dioxane	-	8.55	102.9
2-butanol	-	6.29	96.6
2-methyl-1-propanol	-	5.11	105.0
2-methyl-2-propanol	-	5.30	84.6
2-pentanol	-	4.57	118.8
2-propanol	-	4.99	73.0
2,2,4-trimethylpentane	-	2.33	98.8
3-methyl-1-butanol	-	4.41	131.2
acetone	-	> 9	46.5
benzene	-	4.52	78.8
butanone	-	> 9	75.6
butyl acetate	-	8.05	126.6
carbon disulfide	-	3.03	46.2
carbon tetrachloride	-	3.11	76.0
chloroform	-	4.16	61.2
cyclohexane	-	2.26	80.7
decane	-	1.81	174.9
dibutyl ether	-	4.43	142.1
dichloromethane	-	6.29	39.6
diethyl ether	-	8.68	33.2
DMF	-	4.03	153.0
ethyl acetate	-	> 9	73.9
ethylene glycol	-	3.98	197.5
heptane	-	2.32	98.8
hexadecane	-	1.76	286.6
hexane	-	2.69	68.5
methyl acetate	-	> 9	44.0
methyl tert-butyl ether	-	7.47	55.2
methylcyclohexane	-	2.34	101.1
nonane	-	2.23	151.7
octane	-	2.35	126.4
undecane	-	1.57	196.3
water	-	2.95	100.0

cinnamic acid C₉H₈O₂ - 7 solvents^{72, 902, 48, 907}



Compound Data

Molecular weight	148.159	H bond acceptors	2	Rule of 5 violations	0
Compound type	carboxylic acid	H bond donors	1	ACD/ALogP	2.38
Phase 25°C	solid	Rotatable bonds	2	Predicted density	1.184 g/cm ³
SMILES	O=C(O)C=Cc1ccccc1				
InChIKey	WBYWAXJHAXSJNI-VOTSOKGWSA-N				

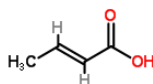
Abraham Solute Descriptors

log S _w	E	S	A	B	V
-2.310	1.161	4.115	0.445	-0.194	0.957

Solubility Data

Solvent	Concentration (M)		Solvent bp °C
	Measured	Predicted	
1-hexanol	0.00	0.03	158.2
chloroform	0.93	0.71	61.2
diethyl ether	0.43	1.07	33.2
ethanol	0.86	0.09	72.6
methanol	1.10	0.46	48.1
toluene	0.30	0.27	110.6
water	0.00	0.00	100
1-butanol	-	0.02	117.7
1-decanol	-	0.00	227.8
1-heptanol	-	0.01	176.9
1-octanol	-	0.06	194.7
1-pentanol	-	0.01	138.5
1-propanol	-	0.04	95.8
1,2-dichloroethane	-	> 9	83.5
1,4-dioxane	-	> 9	102.9
2-butanol	-	0.07	96.6
2-methyl-1-propanol	-	0.03	105.0
2-methyl-2-propanol	-	0.14	84.6
2-pentanol	-	0.00	118.8
2-propanol	-	0.06	73.0
2,2,4-trimethylpentane	-	0.00	98.8
3-methyl-1-butanol	-	0.01	131.2
acetone	-	> 9	46.5
acetonitrile	-	> 9	63.5
benzene	-	0.64	78.8
butanone	-	> 9	75.6
butyl acetate	-	> 9	126.6
carbon disulfide	-	0.08	46.2
carbon tetrachloride	-	0.00	76.0
cyclohexane	-	0.00	80.7
decane	-	0.00	174.9
dibutyl ether	-	0.13	142.1
dichloromethane	-	8.52	39.6
DMF	-	> 9	153.0
DMSO	-	> 9	189.0
ethyl acetate	-	> 9	73.9
ethylene glycol	-	0.07	197.5
heptane	-	0.00	98.8
hexadecane	-	0.00	286.6
hexane	-	0.00	68.5
methyl acetate	-	> 9	44.0
methyl tert-butyl ether	-	0.70	55.2
methylcyclohexane	-	0.00	101.1
nonane	-	0.00	151.7
octane	-	0.00	126.4
THF	-	> 9	68.3
undecane	-	0.00	196.3

crotonic acid C₄H₆O₂ - 10 solvents ^{64, 62, 907}



Compound Data					
Molecular weight	86.0892	H bond acceptors	2	Rule of 5 violations	0
Compound type	carboxylic acid	H bond donors	1	ACD/ALogP	0.94
Phase 25°C	solid	Rotatable bonds	1	Predicted density	1.039 g/cm³
SMILES	O=C(O)/C=C/C				

InChIKey LDHQCZJRKDOVOX-NSCUHMNNSA-N

Abraham Solute Descriptors

log S_w	E	S	A	B	V
-0.051	0.474	0.405	0.130	0.155	0.339

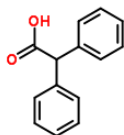
Solubility Data

Solvent	Concentration (M)		Solvent bp °C
	Measured	Predicted	
acetonitrile	3.59	6.14	63.5
benzene	4.45	3.08	78.8
chloroform	7.34	3.70	61.2
DMSO	7.76	6.77	189
ethanol	6.15	5.68	72.6
hexane	1.07	1.43	68.5
methanol	7.62	6.67	48.1
THF	8.09	7.70	68.3
toluene	3.52	2.84	110.6
water	0.89	0.89	100
1-butanol	-	4.32	117.7
1-decanol	-	3.09	227.8
1-heptanol	-	3.20	176.9
1-hexanol	-	3.73	158.2
1-octanol	-	3.13	194.7
1-pentanol	-	3.99	138.5
1-propanol	-	4.74	95.8
1,2-dichloroethane	-	4.04	83.5
1,4-dioxane	-	5.95	102.9
2-butanol	-	4.95	96.6
2-methyl-1-propanol	-	4.30	105.0
2-methyl-2-propanol	-	4.48	84.6
2-pentanol	-	4.09	118.8
2-propanol	-	4.19	73.0
2,2,4-trimethylpentane	-	1.24	98.8
3-methyl-1-butanol	-	3.94	131.2
acetone	-	7.63	46.5
butanone	-	6.90	75.6
butyl acetate	-	5.39	126.6
carbon disulfide	-	1.74	46.2
carbon tetrachloride	-	2.08	76.0
cyclohexane	-	1.27	80.7
decane	-	1.01	174.9
dibutyl ether	-	2.73	142.1
dichloromethane	-	4.74	39.6
diethyl ether	-	5.99	33.2
DMF	-	3.71	153.0
ethyl acetate	-	6.73	73.9
ethylene glycol	-	2.47	197.5
heptane	-	1.36	98.8
hexadecane	-	0.96	286.6
methyl acetate	-	7.18	44.0
methyl tert-butyl ether	-	5.10	55.2
methylcyclohexane	-	1.50	101.1
nonane	-	1.23	151.7
octane	-	1.28	126.4
undecane	-	0.89	196.3

diphenylacetic acid C₁₄H₁₂O₂ - 7 solvents ^{81, 77, 907}

Compound Data

Molecular weight	212.244	H bond acceptors	2	Rule of 5 violations	0
Compound type	carboxylic acid	H bond donors	1	ACD/ALogP	2.79



Phase 25°C solid Rotatable bonds 3 Predicted density 1.174 g/cm³
 SMILES O=C(O)C(c1ccccc1)c2ccccc2
 InChIKey PYHXGXCGESYPCW-UHFFFAOYSA-N

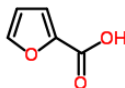
Abraham Solute Descriptors

log S _w	E	S	A	B	V
-2.310	1.565	1.499	0.147	1.083	1.773

Solubility Data

Solvent	Concentration (M)		Solvent bp °C
	Measured	Predicted	
acetonitrile	0.46	0.49	63.5
DMSO	2.56	2.65	189
ethanol	1.15	1.40	72.6
methanol	1.27	1.12	48.1
THF	2.91	2.51	68.3
toluene	0.17	0.93	110.6
water	0.00	0.00	100
1-butanol	-	0.70	117.7
1-decanol	-	0.71	227.8
1-heptanol	-	0.76	176.9
1-hexanol	-	0.79	158.2
1-octanol	-	0.56	194.7
1-pentanol	-	0.81	138.5
1-propanol	-	0.75	95.8
1,2-dichloroethane	-	3.06	83.5
1,4-dioxane	-	2.00	102.9
2-butanol	-	0.90	96.6
2-methyl-1-propanol	-	0.69	105.0
2-methyl-2-propanol	-	0.50	84.6
2-pentanol	-	0.88	118.8
2-propanol	-	0.61	73.0
2,2,4-trimethylpentane	-	0.02	98.8
3-methyl-1-butanol	-	0.81	131.2
acetone	-	1.16	46.5
benzene	-	1.54	78.8
butanone	-	1.59	75.6
butyl acetate	-	0.66	126.6
carbon disulfide	-	0.20	46.2
carbon tetrachloride	-	0.46	76.0
chloroform	-	> 9	61.2
cyclohexane	-	0.06	80.7
decane	-	0.02	174.9
dibutyl ether	-	0.09	142.1
dichloromethane	-	4.75	39.6
diethyl ether	-	0.45	33.2
DMF	-	3.53	153.0
ethyl acetate	-	0.75	73.9
ethylene glycol	-	0.59	197.5
heptane	-	0.03	98.8
hexadecane	-	0.03	286.6
hexane	-	0.02	68.5
methyl acetate	-	1.43	44.0
methyl tert-butyl ether	-	0.33	55.2
methylcyclohexane	-	0.11	101.1
nonane	-	0.03	151.7
octane	-	0.03	126.4
undecane	-	0.02	196.3

furoic acid C₅H₄O₃ - 6 solvents^{104, 911}



Compound Data

Molecular weight	112.084	H bond acceptors	3	Rule of 5 violations	0
Compound type	carboxylic acid	H bond donors	1	ACD/ALogP	0.98
Phase 25°C	solid	Rotatable bonds	1	Predicted density	1.322 g/cm ³
SMILES	OC(=O)c1ccco1				
InChIKey	SMNDYUVBFMFKNZ-UHFFFAOYSA-N				

Abraham Solute Descriptors

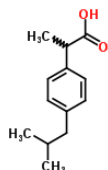
log S _w	E	S	A	B	V
-0.620	0.590	0.351	0.479	0.125	0.366

Solubility Data

Solvent	Concentration (M)		Solvent bp °C
	Measured	Predicted	
acetonitrile	1.10	0.77	63.5
DMSO	6.64	8.41	189
methanol	4.12	3.57	48.1
THF	4.07	3.71	68.3
toluene	0.06	0.16	110.6
water	0.32	0.16	110.6
1-butanol	-	2.79	117.7
1-decanol	-	2.23	227.8
1-heptanol	-	2.08	176.9
1-hexanol	-	2.44	158.2
1-octanol	-	1.88	194.7
1-pentanol	-	2.93	138.5
1-propanol	-	3.80	95.8
1,2-dichloroethane	-	0.22	83.5
1,4-dioxane	-	2.07	102.9
2-butanol	-	3.03	96.6
2-methyl-1-propanol	-	2.79	105.0
2-methyl-2-propanol	-	3.10	84.6
2-pentanol	-	2.93	118.8
2-propanol	-	3.60	73.0
2,2,4-trimethylpentane	-	0.05	98.8
3-methyl-1-butanol	-	2.46	131.2
acetone	-	2.48	46.5
benzene	-	0.16	78.8
butanone	-	1.97	75.6
butyl acetate	-	1.57	126.6
carbon disulfide	-	0.07	46.2
carbon tetrachloride	-	0.08	76.0
chloroform	-	0.15	61.2
cyclohexane	-	0.05	80.7
decane	-	0.05	174.9
dibutyl ether	-	0.53	142.1
dichloromethane	-	0.20	39.6
diethyl ether	-	2.55	33.2
DMF	-	2.34	153.0
ethyl acetate	-	2.20	73.9
ethylene glycol	-	2.18	197.5
heptane	-	0.07	98.8
hexadecane	-	0.04	286.6
hexane	-	0.06	68.5
methyl acetate	-	1.60	44.0
methyl tert-butyl ether	-	1.28	55.2
methylcyclohexane	-	0.07	101.1
nonane	-	0.05	151.7
octane	-	0.06	126.4

undecane	-	0.04	196.3
water	-	0.24	100.0

ibuprofen C₁₃H₁₈O₂ - 10 solvents^{905, 907}



Compound Data

Molecular weight	206.281	H bond acceptors	2	Rule of 5 violations	0
Compound type	carboxylic acid	H bond donors	1	ACD/ALogP	3.5
Phase 25°C	solid	Rotatable bonds	4	Predicted density	1.029 g/cm ³
SMILES	<chem>O=C(O)C(c1ccc(cc1)CC(C)C)C</chem>				
InChIKey	HEFNWNSXXWATRW-UHFFFAOYSA-N				

Abraham Solute Descriptors

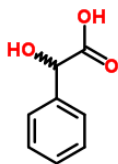
log S _w	E	S	A	B	V
-2.310	0.942	1.122	0.444	1.364	2.061

Solubility Data

Solvent	Concentration (M)		Solvent bp °C
	Measured	Predicted	
1-decanol	1.12	1.10	227.8
1-octanol	1.20	0.70	194.7
1-pentanol	1.46	1.74	138.5
1-propanol	1.52	1.56	95.8
2-butanol	1.78	1.59	96.6
2-methyl-1-propanol	1.76	1.59	105
2-propanol	2.22	1.57	73
ethanol	1.18	2.57	72.6
methanol	1.16	1.57	48.1
water	0.00	0.00	100
1-butanol	-	1.33	117.7
1-heptanol	-	1.44	176.9
1-hexanol	-	1.38	158.2
1,2-dichloroethane	-	0.33	83.5
1,4-dioxane	-	0.62	102.9
2-methyl-2-propanol	-	1.26	84.6
2-pentanol	-	2.39	118.8
2,2,4-trimethylpentane	-	0.00	98.8
3-methyl-1-butanol	-	2.05	131.2
acetone	-	0.34	46.5
acetonitrile	-	0.06	63.5
benzene	-	0.17	78.8
butanone	-	0.47	75.6
butyl acetate	-	0.23	126.6
carbon disulfide	-	0.01	46.2
carbon tetrachloride	-	0.06	76.0
chloroform	-	2.56	61.2
cyclohexane	-	0.01	80.7
decane	-	0.00	174.9
dibutyl ether	-	0.02	142.1
dichloromethane	-	0.74	39.6
diethyl ether	-	0.26	33.2
DMF	-	3.02	153.0
DMSO	-	0.96	189.0
ethyl acetate	-	0.26	73.9
ethylene glycol	-	0.80	197.5
heptane	-	0.01	98.8
hexadecane	-	0.00	286.6
hexane	-	0.00	68.5
methyl acetate	-	0.43	44.0
methyl tert-butyl ether	-	0.15	55.2
methylcyclohexane	-	0.02	101.1
nonane	-	0.00	151.7

octane	-	0.00	126.4
THF	-	1.36	68.3
toluene	-	0.09	110.6
undecane	-	0.00	196.3

mandelic acid C₈H₈O₃ - 5 solvents^{72, 71}



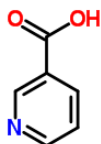
Compound Data			
Molecular weight	152.147	H bond acceptors	3
Compound type	carboxylic acid	H bond donors	2
Phase 25°C	solid	Rotatable bonds	3
SMILES	O=C(O)C(O)c1ccccc1		
InChIKey	IWYDHOAUDWTVEP-UHFFFAOYSA-N		
Rule of 5 violations	0		
ACD/ALogP	0.66		
Predicted density	1.321 g/cm ³		

Abraham Solute Descriptors					
log S _w	E	S	A	B	V
-0.960	0.970	6.447	1.008	-0.527	0.812

Solubility Data			
Concentration (M)			
Solvent	Measured	Predicted	Solvent bp °C
1-hexanol	0.00	0.01	158.2
chloroform	0.12	0.10	61.2
diethyl ether	0.77	1.49	33.2
methanol	3.54	1.13	48.1
toluene	0.00	0.02	110.6
1-butanol	-	0.00	117.7
1-decanol	-	0.00	227.8
1-heptanol	-	0.00	176.9
1-octanol	-	0.02	194.7
1-pentanol	-	0.00	138.5
1-propanol	-	0.02	95.8
1,2-dichloroethane	-	> 9	83.5
1,4-dioxane	-	> 9	102.9
2-butanol	-	0.04	96.6
2-methyl-1-propanol	-	0.01	105.0
2-methyl-2-propanol	-	0.18	84.6
2-pentanol	-	0.00	118.8
2-propanol	-	0.05	73.0
2,2,4-trimethylpentane	-	0.00	98.8
3-methyl-1-butanol	-	0.00	131.2
acetone	-	> 9	46.5
acetonitrile	-	> 9	63.5
benzene	-	0.08	78.8
butanone	-	> 9	75.6
butyl acetate	-	> 9	126.6
carbon disulfide	-	0.00	46.2
carbon tetrachloride	-	0.00	76.0
cyclohexane	-	0.00	80.7
decane	-	0.00	174.9
dibutyl ether	-	0.03	142.1
dichloromethane	-	6.86	39.6
DMF	-	> 9	153.0
DMSO	-	> 9	189.0
ethyl acetate	-	> 9	73.9
ethylene glycol	-	0.21	197.5
heptane	-	0.00	98.8
hexadecane	-	0.00	286.6
hexane	-	0.00	68.5
methyl acetate	-	> 9	44.0
methyl tert-butyl ether	-	0.55	55.2

methylcyclohexane	-	0.00	101.1
nonane	-	0.00	151.7
octane	-	0.00	126.4
THF	-	> 9	68.3
undecane	-	0.00	196.3
water	-	0.11	100.0

nicotinic acid C₆H₅NO₂ - 8 solvents^{100, 137, 907}



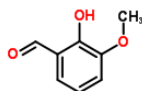
Compound Data			
Molecular weight	123.109	H bond acceptors	3
Compound type	carboxylic acid	H bond donors	1
Phase 25°C	solid	Rotatable bonds	1
SMILES	O=C(O)c1ccncl		
InChIKey	PVNIIMVLHYAWGP-UHFFFAOYSA-N		
Rule of 5 violations	0	ACD/ALogP	0.29
Predicted density	1.293 g/cm ³		

Abraham Solute Descriptors					
log S _w	E	S	A	B	V
-0.432	0.762	0.738	0.461	0.681	0.519

Solubility Data			
Concentration (M)			
Solvent	Measured	Predicted	Solvent bp °C
acetonitrile	0.00	0.02	63.5
benzene	0.00	0.00	78.8
DMSO	0.57	0.28	189
ethanol	0.09	0.11	72.6
methanol	0.06	0.15	48.1
THF	0.06	0.04	68.3
toluene	0.00	0.00	110.6
water	0.37	0.37	100
1-butanol	-	0.05	117.7
1-decanol	-	0.03	227.8
1-heptanol	-	0.03	176.9
1-hexanol	-	0.04	158.2
1-octanol	-	0.03	194.7
1-pentanol	-	0.05	138.5
1-propanol	-	0.07	95.8
1,2-dichloroethane	-	0.01	83.5
1,4-dioxane	-	0.03	102.9
2-butanol	-	0.09	96.6
2-methyl-1-propanol	-	0.06	105.0
2-methyl-2-propanol	-	0.05	84.6
2-pentanol	-	0.06	118.8
2-propanol	-	0.07	73.0
2,2,4-trimethylpentane	-	0.00	98.8
3-methyl-1-butanol	-	0.05	131.2
acetone	-	0.04	46.5
butanone	-	0.03	75.6
butyl acetate	-	0.01	126.6
carbon disulfide	-	0.00	46.2
carbon tetrachloride	-	0.00	76.0
chloroform	-	0.01	61.2
cyclohexane	-	0.00	80.7
decane	-	0.00	174.9
dibutyl ether	-	0.00	142.1
dichloromethane	-	0.01	39.6
diethyl ether	-	0.02	33.2
DMF	-	0.05	153.0
ethyl acetate	-	0.02	73.9
ethylene glycol	-	0.28	197.5
heptane	-	0.00	98.8

hexadecane	-	0.00	286.6
hexane	-	0.00	68.5
methyl acetate	-	0.03	44.0
methyl tert-butyl ether	-	0.01	55.2
methylcyclohexane	-	0.00	101.1
nonane	-	0.00	151.7
octane	-	0.00	126.4
undecane	-	0.00	196.3

o-vanillin C₈H₈O₃ - 5 solvents^{208, 205}



Compound Data				
Molecular weight	152.147	H bond acceptors	3	Rule of 5 violations 0
Compound type	aldehyde	H bond donors	1	ACD/ALogP 1.31
Phase 25°C	solid	Rotatable bonds	3	Predicted density 1.231 g/cm ³
SMILES	Oc1c(cccc1OC)C=O			
InChIKey	JJVNINGBHGJWJH-UHFFFAOYSA-N			

Abraham Solute Descriptors

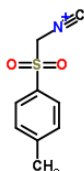
log S _w	E	S	A	B	V
-1.470	1.024	0.802	0.046	0.448	0.935

Solubility Data

Solvent	Concentration (M)		Solvent bp °C
	Measured	Predicted	
acetonitrile	2.56	2.47	63.5
ethanol	3.04	2.74	72.6
methanol	2.27	2.50	48.1
THF	5.37	5.53	68.3
toluene	3.82	3.87	110.6
1-butanol	-	1.96	117.7
1-decanol	-	1.87	227.8
1-heptanol	-	1.86	176.9
1-hexanol	-	1.96	158.2
1-octanol	-	1.61	194.7
1-pentanol	-	2.00	138.5
1-propanol	-	1.97	95.8
1,2-dichloroethane	-	5.84	83.5
1,4-dioxane	-	4.32	102.9
2-butanol	-	2.10	96.6
2-methyl-1-propanol	-	1.77	105.0
2-methyl-2-propanol	-	1.54	84.6
2-pentanol	-	2.02	118.8
2-propanol	-	1.56	73.0
2,2,4-trimethylpentane	-	0.64	98.8
3-methyl-1-butanol	-	1.91	131.2
acetone	-	3.95	46.5
benzene	-	4.64	78.8
butanone	-	4.41	75.6
butyl acetate	-	3.01	126.6
carbon disulfide	-	2.27	46.2
carbon tetrachloride	-	2.71	76.0
chloroform	-	7.93	61.2
cyclohexane	-	1.12	80.7
decane	-	0.57	174.9
dibutyl ether	-	1.16	142.1
dichloromethane	-	7.51	39.6
diethyl ether	-	2.61	33.2
DMF	-	2.98	153.0
DMSO	-	2.98	189.0
ethyl acetate	-	3.40	73.9

ethylene glycol	-	0.83	197.5
heptane	-	0.73	98.8
hexadecane	-	0.64	286.6
hexane	-	0.74	68.5
methyl acetate	-	4.26	44.0
methyl tert-butyl ether	-	2.33	55.2
methylcyclohexane	-	1.38	101.1
nonane	-	0.72	151.7
octane	-	0.78	126.4
undecane	-	0.55	196.3
water	-	0.03	100.0

p-toluenesulfonylmethyl isocyanide C₉H₉NO₂S - 5 solvents²⁰⁸



Compound Data

Molecular weight	195.238	H bond acceptors	3	Rule of 5 violations	0
Compound type	isonitrile	H bond donors	0	ACD/ALogP	1.38
Phase 25°C	solid	Rotatable bonds	2	Predicted density	‡
SMILES	<chem>O=S(=O)(c1ccc(cc1)C)C[N+]#C</chem>				
InChIKey	CFOAUYCPAUGDFF-UHFFFAOYSA-N				

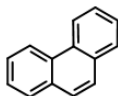
Solubility Data

Solvent	Concentration (M)		Solvent bp °C
	Measured	Predicted	
acetonitrile	1.88	0.03	63.5
chloroform	0.21	0.03	61.2
ethanol	0.18	0.03	72.6
THF	1.86	0.03	68.3
toluene	0.14	0.03	110.6
1-butanol	-	1.96	117.7
1-decanol	-	1.87	227.8
1-heptanol	-	1.86	176.9
1-hexanol	-	1.96	158.2
1-octanol	-	1.61	194.7
1-pentanol	-	2.00	138.5
1-propanol	-	1.97	95.8
1,2-dichloroethane	-	5.84	83.5
1,4-dioxane	-	4.32	102.9
2-butanol	-	2.10	96.6
2-methyl-1-propanol	-	1.77	105.0
2-methyl-2-propanol	-	1.54	84.6
2-pentanol	-	2.02	118.8
2-propanol	-	1.56	73.0
2,2,4-trimethylpentane	-	0.64	98.8
3-methyl-1-butanol	-	1.91	131.2
acetone	-	3.95	46.5
benzene	-	4.64	78.8
butanone	-	4.41	75.6
butyl acetate	-	3.01	126.6
carbon disulfide	-	2.27	46.2
carbon tetrachloride	-	2.71	76.0
cyclohexane	-	1.12	80.7
decane	-	0.57	174.9
dibutyl ether	-	1.16	142.1
dichloromethane	-	7.51	39.6
diethyl ether	-	2.61	33.2
DMF	-	2.98	153.0
DMSO	-	2.98	189.0
ethyl acetate	-	3.40	73.9
ethylene glycol	-	0.83	197.5
heptane	-	0.73	98.8
hexadecane	-	0.64	286.6

hexane	-	0.74	68.5
methanol	-	2.50	48.1
methyl acetate	-	4.26	44.0
methyl tert-butyl ether	-	2.33	55.2
methylcyclohexane	-	1.38	101.1
nonane	-	0.72	151.7
octane	-	0.78	126.4
undecane	-	0.55	196.3
water	-	0.03	100.0

‡ Solute density prediction fail.

phenanthrene C₁₄H₁₀ - 6 solvents⁹⁰²



Compound Data

Molecular weight	178.229	H bond acceptors	0	Rule of 5 violations	0
Compound type	non-Ugi related	H bond donors	0	ACD/ALogP	4.55
Phase 25°C	solid	Rotatable bonds	0	Predicted density	1.13 g/cm ³
SMILES	<chem>c3cc2ccc1ccccc1c2cc3</chem>				
InChIKey	YNPNZTXNASCQKK-UHFFFAOYSA-N				

Abraham Solute Descriptors

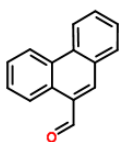
log S _w	E	S	A	B	V
-5.720	2.100	0.840	0.057	0.198	1.435

Solubility Data

Solvent	Concentration (M)		Solvent bp °C
	Measured	Predicted	
benzene	2.02	1.82	78.8
carbon disulfide	3.05	4.78	46.2
carbon tetrachloride	1.73	1.31	76
diethyl ether	1.36	0.91	33.2
ethanol	0.21	0.29	72.6
hexane	0.32	0.31	68.5
1-butanol	-	0.32	117.7
1-decanol	-	0.86	227.8
1-heptanol	-	0.55	176.9
1-hexanol	-	0.44	158.2
1-octanol	-	0.41	194.7
1-pentanol	-	0.44	138.5
1-propanol	-	0.29	95.8
1,2-dichloroethane	-	0.90	83.5
1,4-dioxane	-	1.10	102.9
2-butanol	-	0.18	96.6
2-methyl-1-propanol	-	0.18	105.0
2-methyl-2-propanol	-	0.13	84.6
2-pentanol	-	0.34	118.8
2-propanol	-	0.17	73.0
2,2,4-trimethylpentane	-	0.30	98.8
3-methyl-1-butanol	-	0.27	131.2
acetone	-	0.67	46.5
acetonitrile	-	0.10	63.5
butanone	-	0.88	75.6
butyl acetate	-	0.92	126.6
chloroform	-	0.61	61.2
cyclohexane	-	1.13	80.7
decane	-	0.39	174.9
dibutyl ether	-	0.58	142.1
dichloromethane	-	0.75	39.6
DMF	-	0.43	153.0
DMSO	-	0.27	189.0
ethyl acetate	-	0.90	73.9

ethylene glycol	-	0.02	197.5
heptane	-	0.47	98.8
hexadecane	-	0.40	286.6
methanol	-	0.11	48.1
methyl acetate	-	0.52	44.0
methyl tert-butyl ether	-	0.66	55.2
methylcyclohexane	-	0.89	101.1
nonane	-	0.43	151.7
octane	-	0.58	126.4
THF	-	2.14	68.3
toluene	-	2.09	110.6
undecane	-	0.43	196.3
water	-	0.00	100.0

phenanthrene-9-carboxaldehyde C₁₅H₁₀O - 16 solvents^{30, 60, 136, 4, 242, 51, 24}



Compound Data

Molecular weight	206.239	H bond acceptors	1	Rule of 5 violations	0
Compound type	aldehyde	H bond donors	0	ACD/ALogP	4.28
Phase 25°C	solid	Rotatable bonds	1	Predicted density	1.217 g/cm ³
SMILES	<chem>O=Cc2cc3c(c1c2cccc1)cccc3</chem>				
InChIKey	QECIGCMPORCORE-UHFFFAOYSA-N				

Abraham Solute Descriptors

log S _w	E	S	A	B	V
-5.520	2.494	1.166	0.327	0.423	1.606

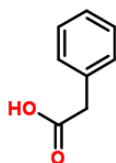
Solubility Data

Solvent	Concentration (M)		Solvent bp °C
	Measured	Predicted	
1,1,2-trichlorotrifluoroethane	0.02	*	50.9
2-propanol	0.07	0.15	73
acetonitrile	0.16	0.03	63.5
benzene	0.66	0.23	78.8
chloroform	0.04	0.10	61.2
cyclohexane	0.07	0.05	80.7
cyclopentane	0.03	*	49.2
dichloromethane	0.00	0.11	39.6
diethyl ether	0.10	0.36	33.2
DMF	1.25	0.50	153
DMSO	0.77	0.83	189
ethanol	0.10	0.26	72.6
hexane	0.07	0.01	68.5
methanol	0.11	0.10	48.1
THF	2.32	1.38	68.3
toluene	0.14	0.24	110.6
1-butanol	-	0.22	117.7
1-decanol	-	0.63	227.8
1-heptanol	-	0.36	176.9
1-hexanol	-	0.31	158.2
1-octanol	-	0.27	194.7
1-pentanol	-	0.34	138.5
1-propanol	-	0.25	95.8
1,2-dichloroethane	-	0.17	83.5
1,4-dioxane	-	0.68	102.9
2-butanol	-	0.15	96.6
2-methyl-1-propanol	-	0.13	105.0
2-methyl-2-propanol	-	0.09	84.6
2-pentanol	-	0.26	118.8
2,2,4-trimethylpentane	-	0.01	98.8
3-methyl-1-butanol	-	0.18	131.2
acetone	-	0.36	46.5

butanone	-	0.43	75.6
butyl acetate	-	0.33	126.6
carbon disulfide	-	0.25	46.2
carbon tetrachloride	-	0.09	76.0
decane	-	0.01	174.9
dibutyl ether	-	0.09	142.1
ethyl acetate	-	0.37	73.9
ethylene glycol	-	0.05	197.5
heptane	-	0.02	98.8
hexadecane	-	0.02	286.6
methyl acetate	-	0.22	44.0
methyl tert-butyl ether	-	0.16	55.2
methylcyclohexane	-	0.05	101.1
nonane	-	0.02	151.7
octane	-	0.02	126.4
undecane	-	0.02	196.3
water	-	0.00	100.0

* This solvent doesn't have recorded Abraham coefficients.

phenylacetic acid C₈H₈O₂ - 7 solvents^{86, 123, 907}



Compound Data

Molecular weight	136.148	H bond acceptors	2	Rule of 5 violations	0
Compound type	carboxylic acid	H bond donors	1	ACD/ALogP	1.72
Phase 25°C	solid	Rotatable bonds	2	Predicted density	1.164 g/cm ³
SMILES	O=C(O)Cc1ccccc1				
InChIKey	WLJVDXDMOQOGPLL-UHFFFAOYSA-N				

Abraham Solute Descriptors

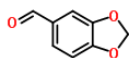
log S _w	E	S	A	B	V
-0.886	0.832	0.917	0.082	0.455	0.837

Solubility Data

Solvent	Concentration (M)		Solvent bp °C
	Measured	Predicted	
acetonitrile	3.87	3.78	63.5
benzene	3.35	3.22	78.8
DMF	3.76	4.39	153
DMSO	6.35	5.83	189
THF	5.62	5.32	68.3
toluene	1.94	2.48	110.6
water	0.13	0.13	100
1-butanol	-	1.67	117.7
1-decanol	-	1.23	227.8
1-heptanol	-	1.41	176.9
1-hexanol	-	1.61	158.2
1-octanol	-	1.34	194.7
1-pentanol	-	1.58	138.5
1-propanol	-	1.79	95.8
1,2-dichloroethane	-	5.41	83.5
1,4-dioxane	-	4.73	102.9
2-butanol	-	2.10	96.6
2-methyl-1-propanol	-	1.70	105.0
2-methyl-2-propanol	-	1.64	84.6
2-pentanol	-	1.64	118.8
2-propanol	-	1.56	73.0
2,2,4-trimethylpentane	-	0.30	98.8
3-methyl-1-butanol	-	1.62	131.2
acetone	-	4.57	46.5
butanone	-	4.98	75.6
butyl acetate	-	2.79	126.6

carbon disulfide	-	1.10	46.2
carbon tetrachloride	-	1.46	76.0
chloroform	-	7.00	61.2
cyclohexane	-	0.46	80.7
decane	-	0.26	174.9
dibutyl ether	-	0.85	142.1
dichloromethane	-	7.10	39.6
diethyl ether	-	2.24	33.2
ethanol	-	2.66	72.6
ethyl acetate	-	3.33	73.9
ethylene glycol	-	1.09	197.5
heptane	-	0.30	98.8
hexadecane	-	0.30	286.6
hexane	-	0.35	68.5
methanol	-	3.01	48.1
methyl acetate	-	4.90	44.0
methyl tert-butyl ether	-	1.99	55.2
methylcyclohexane	-	0.55	101.1
nonane	-	0.33	151.7
octane	-	0.36	126.4
undecane	-	0.25	196.3

piperonal C₈H₆O₃ - 11 solvents ^{71, 30, 907}



Compound Data				
Molecular weight	150.131	H bond acceptors	3	Rule of 5 violations 0
Compound type	aldehyde	H bond donors	0	ACD/ALogP 0.79
Phase 25°C	solid	Rotatable bonds	1	Predicted density 1.337 g/cm ³
SMILES	O=Cc1ccc2OCOc2c1			
InChIKey	SATCULPHIDQDRE-UHFFFAOYSA-N			

Abraham Solute Descriptors

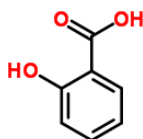
log S _w	E	S	A	B	V
-1.699	1.032	0.928	0.118	0.175	0.769

Solubility Data

Solvent	Concentration (M)		Solvent bp °C
	Measured	Predicted	
acetonitrile	7.11	5.37	63.5
chloroform	7.95	4.22	61.2
dichloromethane	7.59	6.33	39.6
diethyl ether	6.38	4.90	33.2
DMSO	6.05	13.10	189
ethanol	4.99	2.80	72.6
hexane	0.15	0.55	68.5
methanol	7.29	2.71	48.1
THF	7.44	11.41	68.3
toluene	6.40	4.13	110.6
water	0.02	0.02	100
1-butanol	-	2.04	117.7
1-decanol	-	1.83	227.8
1-heptanol	-	1.94	176.9
1-hexanol	-	2.13	158.2
1-octanol	-	2.01	194.7
1-pentanol	-	1.97	138.5
1-propanol	-	2.23	95.8
1,2-dichloroethane	-	6.26	83.5
1,4-dioxane	-	> 9	102.9
2-butanol	-	2.15	96.6
2-methyl-1-propanol	-	1.81	105.0
2-methyl-2-propanol	-	1.92	84.6
2-pentanol	-	1.78	118.8

2-propanol	-	1.83	73.0
2,2,4-trimethylpentane	-	0.49	98.8
3-methyl-1-butanol	-	1.72	131.2
acetone	-	8.95	46.5
benzene	-	4.64	78.8
butanone	-	> 9	75.6
butyl acetate	-	5.91	126.6
carbon disulfide	-	3.33	46.2
carbon tetrachloride	-	1.96	76.0
cyclohexane	-	0.85	80.7
decane	-	0.49	174.9
dibutyl ether	-	2.20	142.1
DMF	-	7.86	153.0
ethyl acetate	-	7.03	73.9
ethylene glycol	-	0.75	197.5
heptane	-	0.48	98.8
hexadecane	-	0.51	286.6
methyl acetate	-	7.65	44.0
methyl tert-butyl ether	-	4.01	55.2
methylcyclohexane	-	0.68	101.1
nonane	-	0.58	151.7
octane	-	0.70	126.4
undecane	-	0.49	196.3

salicylic acid C₇H₆O₃ - 6 solvents^{34, 902, 901, 138, 52, 907}



Compound Data

Molecular weight	138.121	H bond acceptors	3	Rule of 5 violations	0
Compound type	carboxylic acid	H bond donors	2	ACD/ALogP	2.06
Phase 25°C	solid	Rotatable bonds	2	Predicted density	1.375 g/cm ³
SMILES	O=C(O)c1ccccc1O				
InChIKey	YGSDEFSMJLZEOE-UHFFFAOYSA-N				

Abraham Solute Descriptors

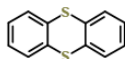
log S _w	E	S	A	B	V
-2.000	0.920	0.110	0.410	0.111	0.595

Solubility Data

Solvent	Concentration (M)		Solvent bp °C
	Measured	Predicted	
chloroform	0.19	0.16	61.2
dichloromethane	0.15	0.18	39.6
ethanol	2.34	3.07	72.6
methanol	2.65	1.89	48.1
toluene	0.11	0.30	110.6
water	0.01	0.01	100
1-butanol	-	3.03	117.7
1-decanol	-	3.98	227.8
1-heptanol	-	2.93	176.9
1-hexanol	-	2.89	158.2
1-octanol	-	2.14	194.7
1-pentanol	-	3.73	138.5
1-propanol	-	3.60	95.8
1,2-dichloroethane	-	0.20	83.5
1,4-dioxane	-	1.34	102.9
2-butanol	-	2.36	96.6
2-methyl-1-propanol	-	2.44	105.0
2-methyl-2-propanol	-	2.24	84.6
2-pentanol	-	3.59	118.8
2-propanol	-	2.89	73.0
2,2,4-trimethylpentane	-	0.16	98.8

3-methyl-1-butanol	-	2.76	131.2
acetone	-	1.43	46.5
acetonitrile	-	0.25	63.5
benzene	-	0.27	78.8
butanone	-	1.22	75.6
butyl acetate	-	1.44	126.6
carbon disulfide	-	0.24	46.2
carbon tetrachloride	-	0.21	76.0
cyclohexane	-	0.22	80.7
decane	-	0.18	174.9
dibutyl ether	-	0.81	142.1
diethyl ether	-	2.76	33.2
DMF	-	0.90	153.0
DMSO	-	1.60	189.0
ethyl acetate	-	1.80	73.9
ethylene glycol	-	0.88	197.5
heptane	-	0.34	98.8
hexadecane	-	0.14	286.6
hexane	-	0.19	68.5
methyl acetate	-	0.94	44.0
methyl tert-butyl ether	-	1.43	55.2
methylcyclohexane	-	0.33	101.1
nonane	-	0.20	151.7
octane	-	0.22	126.4
THF	-	3.21	68.3
undecane	-	0.16	196.3

thianthrene C₁₂H₈S₂ - 10 solvents⁹⁰⁵



Compound Data			
Molecular weight	216.322	H bond acceptors	0
Compound type	non-Ugi related	H bond donors	0
Phase 25°C	solid	Rotatable bonds	0
SMILES	S1c3c(Sc2c1cccc2)cccc3		
InChIKey	GVIIJXMXTUZIOD-UHFFFAOYSA-N		
Rule of 5 violations	0	ACD/ALogP	4.57
		Predicted density	1.31 g/cm ³

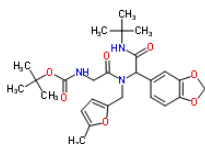
Abraham Solute Descriptors					
log S _w	E	S	A	B	V
-4.290	2.281	1.312	-0.101	0.786	1.543

Solubility Data			
Concentration (M)			
Solvent	Measured	Predicted	Solvent bp °C
1-decanol	0.04	0.08	227.8
1,4-dioxane	0.27	0.16	102.9
acetonitrile	0.02	0.04	63.5
decane	0.03	0.02	174.9
diethyl ether	0.08	0.05	33.2
diisopropyl ether	0.05	*	68.3
ethylene glycol	0.02	0.02	197.5
hexadecane	0.03	0.04	286.6
nonane	0.03	0.03	151.7
undecane	0.03	0.03	196.3
1-butanol	-	0.04	117.7
1-heptanol	-	0.05	176.9
1-hexanol	-	0.05	158.2
1-octanol	-	0.04	194.7
1-pentanol	-	0.05	138.5
1-propanol	-	0.03	95.8
1,2-dichloroethane	-	0.56	83.5
2-butanol	-	0.04	96.6
2-methyl-1-propanol	-	0.03	105.0

2-methyl-2-propanol	-	0.01	84.6
2-pentanol	-	0.04	118.8
2-propanol	-	0.02	73.0
2,2,4-trimethylpentane	-	0.02	98.8
3-methyl-1-butanol	-	0.04	131.2
acetone	-	0.10	46.5
benzene	-	0.55	78.8
butanone	-	0.12	75.6
butyl acetate	-	0.08	126.6
carbon disulfide	-	0.29	46.2
carbon tetrachloride	-	0.29	76.0
chloroform	-	0.88	61.2
cyclohexane	-	0.10	80.7
dibutyl ether	-	0.02	142.1
dichloromethane	-	0.60	39.6
DMF	-	0.06	153.0
DMSO	-	0.06	189.0
ethanol	-	0.06	72.6
ethyl acetate	-	0.08	73.9
heptane	-	0.03	98.8
hexane	-	0.03	68.5
methanol	-	0.04	48.1
methyl acetate	-	0.11	44.0
methyl tert-butyl ether	-	0.04	55.2
methylcyclohexane	-	0.13	101.1
octane	-	0.04	126.4
THF	-	0.18	68.3
toluene	-	0.43	110.6
water	-	0.00	100.0

* This solvent doesn't have recorded Abraham coefficients.

UCExp216-3A C₂₆H₃₅N₃O₇ - 5 solvents¹¹³



Compound Data					
Molecular weight	501.572	H bond acceptors	10	Rule of 5 violations	2
Compound type	Ugi Product	H bond donors	2	ACD/ALogP	4.06
Phase 25°C	solid	Rotatable bonds	10	Predicted density	1.209 g/cm ³
SMILES	<chem>CC(C)(C)NC(=O)C(c1ccc2OCOc2c1)N(Cc3ccc(C)oc3)C(=O)CNC(=O)OC(C)(C)C</chem>				
InChIKey	MTSJLRXXXJHLDI-UHFFFAOYSA-N				

Abraham Solute Descriptors

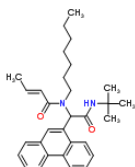
log S _w	E	S	A	B	V
-4.050	2.332	4.791	-0.007	3.981	5.203

Solubility Data

Solvent	Concentration (M)		Solvent bp °C
	Measured	Predicted	
acetonitrile	0.04	0.01	63.5
DMSO	0.28	0.52	189
ethanol	0.03	0.03	72.6
methanol	0.06	0.03	48.1
toluene	0.01	0.02	110.6
1-butanol	-	0.00	117.7
1-decanol	-	0.00	227.8
1-heptanol	-	0.00	176.9
1-hexanol	-	0.00	158.2
1-octanol	-	0.00	194.7
1-pentanol	-	0.00	138.5
1-propanol	-	0.00	95.8

1,2-dichloroethane	-	7.32	83.5
1,4-dioxane	-	0.09	102.9
2-butanol	-	0.01	96.6
2-methyl-1-propanol	-	0.01	105.0
2-methyl-2-propanol	-	0.00	84.6
2-pentanol	-	0.00	118.8
2-propanol	-	0.00	73.0
2,2,4-trimethylpentane	-	0.00	98.8
3-methyl-1-butanol	-	0.01	131.2
acetone	-	0.01	46.5
benzene	-	0.22	78.8
butanone	-	0.05	75.6
butyl acetate	-	0.00	126.6
carbon disulfide	-	0.00	46.2
carbon tetrachloride	-	0.00	76.0
chloroform	-	> 9	61.2
cyclohexane	-	0.00	80.7
decane	-	0.00	174.9
dibutyl ether	-	0.00	142.1
dichloromethane	-	> 9	39.6
diethyl ether	-	0.00	33.2
DMF	-	> 9	153.0
ethyl acetate	-	0.00	73.9
ethylene glycol	-	0.03	197.5
heptane	-	0.00	98.8
hexadecane	-	0.00	286.6
hexane	-	0.00	68.5
methyl acetate	-	0.06	44.0
methyl tert-butyl ether	-	0.00	55.2
methylcyclohexane	-	0.00	101.1
nonane	-	0.00	151.7
octane	-	0.00	126.4
THF	-	0.04	68.3
undecane	-	0.00	196.3
water	-	0.00	100.0

Ugi product 148B C₃₁H₄₀N₂O₂ - 6 solvents^{145, 96}



Compound Data

Molecular weight	472.661	H bond acceptors	4	Rule of 5 violations	1
Compound type	Ugi Product	H bond donors	1	ACD/ALogP	7.47
Phase 25°C	solid	Rotatable bonds	11	Predicted density	1.067 g/cm ³
SMILES	<chem>CC(C)(C)NC(=O)C(N(CCCCCC)C(=O)C=C)C2CC3CCCC3C1CCCC12</chem>				
InChIKey	HOKCUULFCASQT-FRKPEAEDSA-N				

Abraham Solute Descriptors

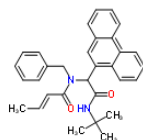
log S _w	E	S	A	B	V
-7.620	3.440	5.683	0.240	3.436	5.615

Solubility Data

Solvent	Concentration (M)		Solvent bp °C
	Measured	Predicted	
acetonitrile	0.02	0.02	63.5
benzene	0.05	0.24	78.8
ethanol	0.00	0.01	72.6
methanol	0.03	0.01	48.1
THF	0.40	0.39	68.3
toluene	0.14	0.03	110.6
1-butanol	-	0.00	117.7
1-decanol	-	0.00	227.8
1-heptanol	-	0.00	176.9
1-hexanol	-	0.00	158.2

1-octanol	-	0.00	194.7
1-pentanol	-	0.00	138.5
1-propanol	-	0.00	95.8
1,2-dichloroethane	-	7.34	83.5
1,4-dioxane	-	0.83	102.9
2-butanol	-	0.00	96.6
2-methyl-1-propanol	-	0.00	105.0
2-methyl-2-propanol	-	0.00	84.6
2-pentanol	-	0.00	118.8
2-propanol	-	0.00	73.0
2,2,4-trimethylpentane	-	0.00	98.8
3-methyl-1-butanol	-	0.00	131.2
acetone	-	0.05	46.5
butanone	-	0.30	75.6
butyl acetate	-	0.01	126.6
carbon disulfide	-	0.00	46.2
carbon tetrachloride	-	0.00	76.0
chloroform	-	> 9	61.2
cyclohexane	-	0.00	80.7
decane	-	0.00	174.9
dibutyl ether	-	0.00	142.1
dichloromethane	-	> 9	39.6
diethyl ether	-	0.00	33.2
DMF	-	> 9	153.0
DMSO	-	> 9	189.0
ethyl acetate	-	0.01	73.9
ethylene glycol	-	0.00	197.5
heptane	-	0.00	98.8
hexadecane	-	0.00	286.6
hexane	-	0.00	68.5
methyl acetate	-	0.14	44.0
methyl tert-butyl ether	-	0.00	55.2
methylcyclohexane	-	0.00	101.1
nonane	-	0.00	151.7
octane	-	0.00	126.4
undecane	-	0.00	196.3
water	-	0.00	100.0

Ugi product 150D(UC) C₃₁H₃₂N₂O₂ - 6 solvents^{78, 65}



Compound Data

Molecular weight	464.598	H bond acceptors	4	Rule of 5 violations	1
Compound type	Ugi Product	H bond donors	1	ACD/ALogP	6.18
Phase 25°C	solid	Rotatable bonds	7	Predicted density	1.148 g/cm ³
SMILES	<chem>CC(C)(C)NC(=O)C(N(Cc1ccccc1)C(=O))C=C(C)c3cc4ccccc4c2ccccc23</chem>				
InChIKey	PBZQTKRWYXTXIS-WLRTZDKTSA-N				

Abraham Solute Descriptors

log S _w	E	S	A	B	V
-7.160	4.342	4.362	0.051	3.236	5.052

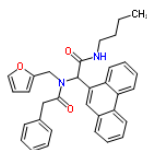
Solubility Data

Concentration (M)

Solvent	Measured	Predicted	Solvent bp °C
acetonitrile	0.04	0.01	63.5
DMSO	0.18	0.74	189
ethanol	0.04	0.05	72.6
methanol	0.07	0.02	48.1
THF	0.49	0.27	68.3
toluene	0.04	0.21	110.6
1-butanol	-	0.01	117.7

1-decanol	-	0.02	227.8
1-heptanol	-	0.02	176.9
1-hexanol	-	0.02	158.2
1-octanol	-	0.01	194.7
1-pentanol	-	0.01	138.5
1-propanol	-	0.01	95.8
1,2-dichloroethane	-	6.33	83.5
1,4-dioxane	-	0.34	102.9
2-butanol	-	0.02	96.6
2-methyl-1-propanol	-	0.01	105.0
2-methyl-2-propanol	-	0.00	84.6
2-pentanol	-	0.02	118.8
2-propanol	-	0.01	73.0
2,2,4-trimethylpentane	-	0.00	98.8
3-methyl-1-butanol	-	0.01	131.2
acetone	-	0.03	46.5
benzene	-	0.99	78.8
butanone	-	0.11	75.6
butyl acetate	-	0.01	126.6
carbon disulfide	-	0.00	46.2
carbon tetrachloride	-	0.03	76.0
chloroform	-	> 9	61.2
cyclohexane	-	0.00	80.7
decane	-	0.00	174.9
dibutyl ether	-	0.00	142.1
dichloromethane	-	> 9	39.6
diethyl ether	-	0.00	33.2
DMF	-	5.21	153.0
ethyl acetate	-	0.01	73.9
ethylene glycol	-	0.03	197.5
heptane	-	0.00	98.8
hexadecane	-	0.00	286.6
hexane	-	0.00	68.5
methyl acetate	-	0.07	44.0
methyl tert-butyl ether	-	0.00	55.2
methylcyclohexane	-	0.00	101.1
nonane	-	0.00	151.7
octane	-	0.00	126.4
undecane	-	0.00	196.3
water	-	0.00	100.0

Ugi product 176C (UC) C₃₃H₃₂N₂O₃ - 11 solvents^{155, 127, 144}



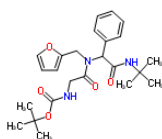
Compound Data				
Molecular weight	504.619	H bond acceptors	5	Rule of 5 violations 2
Compound type	Ugi Product	H bond donors	1	ACD/ALogP 6.9
Phase 25°C	solid	Rotatable bonds	10	Predicted density 1.197 g/cm ³
SMILES	<chem>O=C(Cc1ccccc1)N(Cc2ccco2)C(c4cc5ccccc5c3ccccc34)C(=O)NCCCC</chem>			
InChIKey	RGGYLRDGAJICY-UHFFFAOYSA-N			

Abraham Solute Descriptors					
log S _w	E	S	A	B	V
-5.310	4.713	4.490	0.151	3.935	5.298

Solubility Data			
Concentration (M)			
Solvent	Measured	Predicted	Solvent bp °C
1-octanol	0.01	0.01	194.7
1,4-dioxane	0.19	0.12	102.9
acetonitrile	0.02	0.00	63.5
benzene	0.03	0.33	78.8
diethyl ether	0.02	0.00	33.2

DMF	0.27	2.14	153
DMSO	0.19	0.53	189
ethanol	0.01	0.10	72.6
methanol	0.02	0.05	48.1
THF	0.28	0.10	68.3
toluene	0.03	0.05	110.6
1-butanol	-	0.01	117.7
1-decanol	-	0.03	227.8
1-heptanol	-	0.02	176.9
1-hexanol	-	0.02	158.2
1-pentanol	-	0.02	138.5
1-propanol	-	0.01	95.8
1,2-dichloroethane	-	3.14	83.5
2-butanol	-	0.03	96.6
2-methyl-1-propanol	-	0.01	105.0
2-methyl-2-propanol	-	0.00	84.6
2-pentanol	-	0.03	118.8
2-propanol	-	0.01	73.0
2,2,4-trimethylpentane	-	0.00	98.8
3-methyl-1-butanol	-	0.03	131.2
acetone	-	0.01	46.5
butanone	-	0.03	75.6
butyl acetate	-	0.00	126.6
carbon disulfide	-	0.00	46.2
carbon tetrachloride	-	0.01	76.0
chloroform	-	> 9	61.2
cyclohexane	-	0.00	80.7
decane	-	0.00	174.9
dibutyl ether	-	0.00	142.1
dichloromethane	-	> 9	39.6
ethyl acetate	-	0.00	73.9
ethylene glycol	-	0.34	197.5
heptane	-	0.00	98.8
hexadecane	-	0.00	286.6
hexane	-	0.00	68.5
methyl acetate	-	0.03	44.0
methyl tert-butyl ether	-	0.00	55.2
methylcyclohexane	-	0.00	101.1
nonane	-	0.00	151.7
octane	-	0.00	126.4
undecane	-	0.00	196.3
water	-	0.00	100.0

Ugi product 206B(UC) C₂₄H₃₃N₃O₅ - 16 solvents⁵⁶



Compound Data			
Molecular weight	443.536	H bond acceptors	8
Compound type	Ugi Product	H bond donors	2
Phase 25°C	solid	Rotatable bonds	10
SMILES	O=C(CNC(=O)OC(C)(C)C)N(Cc1ccccc1)C(c2ccccc2)C(=O)NC(C)(C)C		
InChIKey	BXAOUWIVXLQYOZ-UHFFFAOYSA-N		

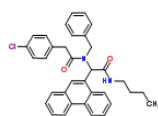
Abraham Solute Descriptors					
log S _w	E	S	A	B	V
-4.240	1.915	2.463	0.301	3.663	4.800

Solubility Data			
Concentration (M)			
Solvent	Measured	Predicted	Solvent bp °C
2-propanol	0.00	0.18	73.0
acetonitrile	0.02	0.00	63.5

benzene	0.01	0.11	78.8
carbon tetrachloride	0.00	0.02	76
chloroform	0.57	279.75	61.2
cyclohexane	0.00	0.00	80.7
cyclopentane	0.00	*	49.2
dichloromethane	0.24	4.64	39.6
diethyl ether	0.00	0.00	33.2
DMF	0.24	1.01	153
DMSO	0.23	0.01	189
ethanol	0.02	0.88	72.6
hexane	0.00	0.00	68.5
methanol	0.05	0.30	48.1
THF	0.26	0.08	68.3
toluene	0.01	0.02	110.6
1-butanol	-	0.20	117.7
1-decanol	-	0.21	227.8
1-heptanol	-	0.36	176.9
1-hexanol	-	0.26	158.2
1-octanol	-	0.07	194.7
1-pentanol	-	0.39	138.5
1-propanol	-	0.18	95.8
1,2-dichloroethane	-	0.48	83.5
1,4-dioxane	-	0.03	102.9
2-butanol	-	0.35	96.6
2-methyl-1-propanol	-	0.32	105.0
2-methyl-2-propanol	-	0.11	84.6
2-pentanol	-	0.94	118.8
2,2,4-trimethylpentane	-	0.00	98.8
3-methyl-1-butanol	-	0.79	131.2
acetone	-	0.00	46.5
butanone	-	0.02	75.6
butyl acetate	-	0.00	126.6
carbon disulfide	-	0.00	46.2
decane	-	0.00	174.9
dibutyl ether	-	0.00	142.1
ethyl acetate	-	0.00	73.9
ethylene glycol	-	0.28	197.5
heptane	-	0.00	98.8
hexadecane	-	0.00	286.6
methyl acetate	-	0.02	44.0
methyl tert-butyl ether	-	0.00	55.2
methylcyclohexane	-	0.00	101.1
nonane	-	0.00	151.7
octane	-	0.00	126.4
undecane	-	0.00	196.3
water	-	0.00	100.0

* This solvent doesn't have recorded Abraham coefficients.

Ugi product 215F(UC) C₃₅H₃₃ClN₂O₂ - 6 solvents⁷¹



Compound Data

Molecular weight	549.102	H bond acceptors	4	Rule of 5 violations	2
Compound type	Ugi Product	H bond donors	1	ACD/ALogP	8.33
Phase 25°C	solid	Rotatable bonds	10	Predicted density	1.219 g/cm ³
SMILES	<chem>Clc5ccc(CC(=O)N(Cc1ccccc1)C(c3cc4ccccc4c2ccccc23)C(=O)NCCCC)cc5</chem>				
InChIKey	NCOSMKWGNJCPCR-UHFFFAOYSA-N				

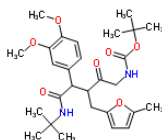
Abraham Solute Descriptors

log S _w	E	S	A	B	V
-7.580	5.307	4.975	0.047	3.742	5.726

Solubility Data

Solvent	Concentration (M)		Solvent bp °C
	Measured	Predicted	
acetonitrile	0.04	0.00	63.5
DMSO	0.38	1.63	189
ethanol	0.06	0.08	72.6
methanol	0.12	0.03	48.1
THF	0.61	0.44	68.3
toluene	0.07	0.41	110.6
1-butanol	-	0.01	117.7
1-decanol	-	0.03	227.8
1-heptanol	-	0.03	176.9
1-hexanol	-	0.02	158.2
1-octanol	-	0.01	194.7
1-pentanol	-	0.02	138.5
1-propanol	-	0.01	95.8
1,2-dichloroethane	-	> 9	83.5
1,4-dioxane	-	0.58	102.9
2-butanol	-	0.02	96.6
2-methyl-1-propanol	-	0.01	105.0
2-methyl-2-propanol	-	0.00	84.6
2-pentanol	-	0.02	118.8
2-propanol	-	0.01	73.0
2,2,4-trimethylpentane	-	0.00	98.8
3-methyl-1-butanol	-	0.02	131.2
acetone	-	0.04	46.5
benzene	-	2.33	78.8
butanone	-	0.15	75.6
butyl acetate	-	0.01	126.6
carbon disulfide	-	0.00	46.2
carbon tetrachloride	-	0.05	76.0
chloroform	-	> 9	61.2
cyclohexane	-	0.00	80.7
decane	-	0.00	174.9
dibutyl ether	-	0.00	142.1
dichloromethane	-	> 9	39.6
diethyl ether	-	0.00	33.2
DMF	-	> 9	153.0
ethyl acetate	-	0.01	73.9
ethylene glycol	-	0.08	197.5
heptane	-	0.00	98.8
hexadecane	-	0.00	286.6
hexane	-	0.00	68.5
methyl acetate	-	0.09	44.0
methyl tert-butyl ether	-	0.00	55.2
methylcyclohexane	-	0.00	101.1
nonane	-	0.00	151.7
octane	-	0.00	126.4
undecane	-	0.00	196.3
water	-	0.00	100.0

Ugi Product 216-4A C₂₈H₄₀N₂O₇ - 5 solvents^{97, 93}



Compound Data

Molecular weight	516.626	H bond acceptors	9	Rule of 5 violations	1
Compound type	Ugi Product	H bond donors	2	ACD/ALogP	4.08
Phase 25°C	solid	Rotatable bonds	13	Predicted density	1.12 g/cm ³
SMILES	<chem>Cc1ccc(o1)CC(C(c2ccc(c(c2)OC)OC)C(=O)NC(C)(C)C)C(=O)CNC(=O)OC(C)(C)C</chem>				
InChIKey					

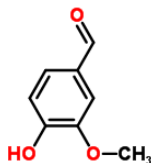
Abraham Solute Descriptors

log S _w	E	S	A	B	V
-4.630	1.716	4.742	-0.317	4.359	5.883

Solubility Data

Solvent	Concentration (M)		Solvent bp °C
	Measured	Predicted	
acetonitrile	0.13	0.04	63.5
DMSO	0.06	0.12	189
ethanol	0.07	0.08	72.6
methanol	0.18	0.08	48.1
toluene	0.20	0.46	110.6
1-butanol	-	0.01	117.7
1-decanol	-	0.00	227.8
1-heptanol	-	0.01	176.9
1-hexanol	-	0.01	158.2
1-octanol	-	0.00	194.7
1-pentanol	-	0.01	138.5
1-propanol	-	0.01	95.8
1,2-dichloroethane	-	> 9	83.5
1,4-dioxane	-	0.23	102.9
2-butanol	-	0.03	96.6
2-methyl-1-propanol	-	0.02	105.0
2-methyl-2-propanol	-	0.01	84.6
2-pentanol	-	0.02	118.8
2-propanol	-	0.01	73.0
2,2,4-trimethylpentane	-	0.00	98.8
3-methyl-1-butanol	-	0.03	131.2
acetone	-	0.02	46.5
benzene	-	5.40	78.8
butanone	-	0.14	75.6
butyl acetate	-	0.00	126.6
carbon disulfide	-	0.00	46.2
carbon tetrachloride	-	0.17	76.0
chloroform	-	> 9	61.2
cyclohexane	-	0.00	80.7
decane	-	0.00	174.9
dibutyl ether	-	0.00	142.1
dichloromethane	-	> 9	39.6
diethyl ether	-	0.00	33.2
DMF	-	> 9	153.0
ethyl acetate	-	0.00	73.9
ethylene glycol	-	0.01	197.5
heptane	-	0.00	98.8
hexadecane	-	0.00	286.6
hexane	-	0.00	68.5
methyl acetate	-	0.23	44.0
methyl tert-butyl ether	-	0.00	55.2
methylcyclohexane	-	0.00	101.1
nonane	-	0.00	151.7
octane	-	0.00	126.4
THF	-	0.12	68.3
undecane	-	0.00	196.3
water	-	0.00	100.0

vanillin C₈H₈O₃ - 8 solvents^{906, 4, 55, 11, 10, 207, 19}



Compound Data

Molecular weight	152.147	H bond acceptors	3	Rule of 5 violations	0
Compound type	aldehyde	H bond donors	1	ACD/ALogP	1.19
Phase 25°C	solid	Rotatable bonds	3	Predicted density	1.231 g/cm ³
SMILES	<chem>Oc1ccc(cc1OC)C=O</chem>				

InChIKey MWOOGJBHARFG-UHFFFAOYSA-N

Abraham Solute Descriptors

log S_w	E	S	A	B	V
-1.480	1.024	1.086	0.365	0.411	0.935

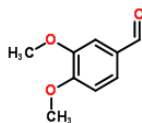
Solubility Data

Solvent	Concentration (M)		Solvent bp °C
	Measured	Predicted	
1-propanol	1.82	1.73	95.8
1,2-dichloroethane	1.17	0.95	83.5
acetonitrile	2.36	1.36	63.5
butanone	2.14	3.49	75.6
ethanol	2.47	2.22	72.6
methanol	4.16	2.22	48.1
THF	3.59	5.31	68.3
toluene	0.30	0.39	110.6
1-butanol	-	1.32	117.7
1-decanol	-	1.03	227.8
1-heptanol	-	1.16	176.9
1-hexanol	-	1.34	158.2
1-octanol	-	1.11	194.7
1-pentanol	-	1.35	138.5
1,4-dioxane	-	3.97	102.9
2-butanol	-	1.64	96.6
2-methyl-1-propanol	-	1.35	105.0
2-methyl-2-propanol	-	1.46	84.6
2-pentanol	-	1.31	118.8
2-propanol	-	1.60	73.0
2,2,4-trimethylpentane	-	0.02	98.8
3-methyl-1-butanol	-	1.20	131.2
acetone	-	3.39	46.5
benzene	-	0.50	78.8
butyl acetate	-	1.70	126.6
carbon disulfide	-	0.14	46.2
carbon tetrachloride	-	0.13	76.0
chloroform	-	0.81	61.2
cyclohexane	-	0.04	80.7
decane	-	0.02	174.9
dibutyl ether	-	0.32	142.1
dichloromethane	-	0.97	39.6
diethyl ether	-	1.62	33.2
DMF	-	7.11	153.0
DMSO	-	> 9	189.0
ethyl acetate	-	2.24	73.9
ethylene glycol	-	1.09	197.5
heptane	-	0.02	98.8
hexadecane	-	0.02	286.6
hexane	-	0.02	68.5
methyl acetate	-	2.57	44.0
methyl tert-butyl ether	-	0.94	55.2
methylcyclohexane	-	0.04	101.1
nonane	-	0.03	151.7
octane	-	0.03	126.4
undecane	-	0.02	196.3
water	-	0.03	100.0

veratraldehyde C₉H₁₀O₃ - 11 solvents^{41, 71, 208}

Compound Data

Molecular weight	166.174	H bond acceptors	3	Rule of 5 violations	0
Compound type	aldehyde	H bond donors	0	ACD/ALogP	1.61



Phase 25°C solid Rotatable bonds 3 Predicted density 1.114 g/cm³
 SMILES COc1cc(ccc1OC)C=O
 InChIKey WJUFSDZVCOTFON-UHFFFAOYSA-N

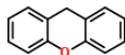
Abraham Solute Descriptors

log S _w	E	S	A	B	V
-2.080	0.889	1.091	0.204	0.572	1.310

Solubility Data

Concentration (M)

Solvent	Measured	Predicted	Solvent bp °C
acetone	3.03	5.03	46.5
acetonitrile	5.76	2.16	63.5
chloroform	5.70	7.59	61.2
dichloromethane	6.06	6.76	39.6
diethyl ether	3.55	2.82	33.2
DMSO	5.31	8.78	189
ethanol	5.49	3.51	72.6
hexane	0.07	0.14	68.5
methanol	5.87	2.90	48.1
THF	5.33	9.71	68.3
toluene	4.54	2.14	110.6
1-butanol	-	2.27	117.7
1-decanol	-	1.80	227.8
1-heptanol	-	2.37	176.9
1-hexanol	-	2.44	158.2
1-octanol	-	1.91	194.7
1-pentanol	-	2.36	138.5
1-propanol	-	2.51	95.8
1,2-dichloroethane	-	4.69	83.5
1,4-dioxane	-	6.79	102.9
2-butanol	-	2.48	96.6
2-methyl-1-propanol	-	2.31	105.0
2-methyl-2-propanol	-	2.43	84.6
2-pentanol	-	2.47	118.8
2-propanol	-	2.28	73.0
2,2,4-trimethylpentane	-	0.12	98.8
3-methyl-1-butanol	-	2.41	131.2
benzene	-	2.89	78.8
butanone	-	6.44	75.6
butyl acetate	-	3.36	126.6
carbon disulfide	-	0.86	46.2
carbon tetrachloride	-	1.04	76.0
cyclohexane	-	0.23	80.7
decane	-	0.13	174.9
dibutyl ether	-	0.82	142.1
DMF	-	> 9	153.0
ethyl acetate	-	3.80	73.9
ethylene glycol	-	0.69	197.5
heptane	-	0.15	98.8
hexadecane	-	0.13	286.6
methyl acetate	-	5.14	44.0
methyl tert-butyl ether	-	2.26	55.2
methylcyclohexane	-	0.29	101.1
nonane	-	0.15	151.7
octane	-	0.17	126.4
undecane	-	0.13	196.3
water	-	0.01	100.0

xanthene C₁₃H₁₀O - 37 solvents⁹⁰⁵

Compound Data				
Molecular weight	182.218	H bond acceptors	1	Rule of 5 violations 0
Compound type	non-Ugi related	H bond donors	0	ACD/ALogP 3.93
Phase 25°C	solid	Rotatable bonds	0	Predicted density 1.159 g/cm ³
SMILES	O2c1ccccc1Cc3c2ccccc3			
InChIKey	GJCOSYZMQJWQCA-UHFFFAOYSA-N			

Abraham Solute Descriptors					
log S _w	E	S	A	B	V
-4.270	1.517	1.171	-0.085	0.454	1.428

Solubility Data			
Concentration (M)			
Solvent	Measured	Predicted	Solvent bp °C
1-butanol	0.19	0.18	117.7
1-decanol	0.24	0.24	227.8
1-heptanol	0.23	0.24	176.9
1-hexanol	0.22	0.22	158.2
1-octanol	0.24	0.21	194.7
1-pentanol	0.20	0.20	138.5
1-propanol	0.15	0.16	95.8
1,2-dichloroethane	1.62	2.87	83.5
2-butanol	0.13	0.16	96.6
2-methyl-1-pentanol	0.16	*	148
2-methyl-1-propanol	0.12	0.14	105
2-methyl-2-butanol	0.18	*	102
2-methyl-2-propanol	0.12	0.12	84.6
2-pentanol	0.16	0.18	118.8
2-propanol	0.11	0.11	73
2,2,4-trimethylpentane	0.15	0.18	98.8
3-methyl-1-butanol	0.15	0.17	131.2
4-methyl-2-pentanol	0.14	*	133.5
acetonitrile	0.35	0.38	63.5
carbon tetrachloride	1.25	1.49	76
cyclohexane	0.39	0.53	80.7
cyclooctane	0.38	*	152
cyclopentanol	0.33	*	140.8
decane	0.24	0.19	174.9
dibutyl ether	0.50	0.30	142.1
diethyl ether	0.79	0.47	33.2
diisopropyl ether	0.41	*	68.3
ethanol	0.10	0.23	72.6
heptane	0.24	0.19	98.8
hexadecane	0.24	0.23	286.6
hexane	0.23	0.20	68.5
methanol	0.10	0.16	48.1
methyl tert-butyl ether	0.65	0.48	55.2
methylcyclohexane	0.33	0.45	101.1
nonane	0.24	0.23	151.7
octane	0.25	0.28	126.4
undecane	0.23	0.21	196.3

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