

Finding chemical and physical property data

There are so many sources of chemical and physical property data that it's difficult to know where to start. This guide highlights a few of the resources that we have available through the University of Bath Library plus a few key open access resources. The resources are all listed on the library webpage for chemistry:

<http://www.bath.ac.uk/library/subjects/chem/index.html>

Measurements of physical and chemical properties are often done by researchers in academic institutions and published in the journal literature. Governments and chemical companies also produce property data. Individual measurements may vary due to factors such as temperature, pressure and purity of the substance. For common substances, properties will have been measured many times and an 'accepted value' will be entered into a data compendium. These are the best places to start your search.

Merck Index

Hosted by the RSC, it contains information on over 11,500 substances. Includes melting point, boiling point, density and solubility. Also gives the chemical structure and literature references to synthesis and bioactivity. Search by name, formula, CAS registry number or structure.

THE
MERCK INDEX Online



Home	Search	Structure Search	Named Reactions	Reference Tables	My Records	Help
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Home > Monograph

Aspirin Print view Add to My Records

Monograph ID:	MONO1500000841
Title:	Aspirin
CAS Registry Number:	50-78-2
CAS Name:	2-(Acetyloxy)benzoic acid
Additional Names:	salicylic acid acetate, 2-acetoxybenzoic acid, acetylsalicylic acid
Trademark Names:	Acylpyrin (Slovakofarma), Angettes (BMS), Asatard (Boehringer, Ing.), Aspro (Roche), Cardioaspirin (Bayer), Cardiprin (Reckitt Benckiser), Cemirit (Bayer), Claragine (Nicholas), Ecotrin (GSK), Empririn (GSK), Encaprin (Procter & Gamble), Rhonal (Aventis), Solprin (Reckitt Benckiser)
Molecular Formula:	C ₉ H ₈ O ₄
Molecular Weight:	180.16
Percent Composition:	C 60.00%, H 4.48%, O 35.52%
Standard InChI:	InChI=1S/C9H8O4/c1-6(10)13-8-5-3-2-4-7(8)9(11)12/h2-5H,1H3,(H,11,12)
Standard InChIKey:	BSYNRYMUTXBXSQ-UHFFFAOYSA-N

Save

Image Structure Zoom

RSC Content

Powered by ChemSpider

- ChemSpider Record
- ChemSpider Name Search
- ChemSpider Skeleton Search
- Search RSC Platform

Properties

White monoclinic tablets or needle-like crystals. *d* 1.40. mp 135°C (rapid heating); the melt solidifies at 118°. uv max (0.1N H₂SO₄): 229 nm (E^{1%_{1cm} 484); (CHCl₃): 277 nm (E^{1%_{1cm} 68). Is odorless, but in moist air it is gradually hydrolyzed into salicylic and acetic acids and acquires the odor of acetic acid. Stable in dry air. pK (25°) 3.49. One gram dissolves in 300 ml water at 25°, in 100 ml water at 37°, in 5 ml alcohol, 17 ml chloroform, 10-15 ml ether. Less soluble in anhydrous ether. Decomposes by boiling water or when dissolved in solutions of alkali hydroxides and carbonates. Inorganic salts of acetylsalicylic acid are soluble in water (esp the Ca salt, *q.v.*), but are decomposed quickly. LD₅₀ orally in mice, rats: 1.1, 1.5 g/kg (Hart).}}

Combined Chemical Dictionary

An online database containing information on over 500,000 substances from the well-known printed Dictionaries of Organic Compounds, Inorganic and Organometallic Compounds, Analytical Reagents, Carbohydrates, Drugs and Natural Products. Search by name, formula, CAS Registry number or structure. It includes melting and boiling points, density, refractive index and journal references to synthesis and spectra.

Boolean	Property	Comparison	Value
AND	Chemical Name		benzoic acid [browse...] [clear]
AND	Molecular Formula		<input type="text"/> [browse...] [clear]
AND	Molecular Formula by Element	= <input type="text"/> C <input type="text"/>	<input type="text"/> [clear]
AND	CAS Registry Nos.		<input type="text"/> [browse...] [clear]
AND	All Text		<input type="text"/> [browse...] [clear]
AND	Melting Point	= <input type="text"/>	<input type="text"/> [browse...] [clear]
AND	Boiling Point	= <input type="text"/>	<input type="text"/> [browse...] [clear]

[Search](#) [View Results in New Window](#)

CRC Handbook of Chemistry and Physics

Contains information on approximately 11,000 substances, including melting point, boiling point, density, solubility and refractive index. It's available in print and online, but is not the easiest source to search. When using the print version, look up at the *property* in the index: for organic compounds you will find a table called 'Physical constants of organic compounds' which lists the substances alphabetically. When using the online version, use the *structure/property* search and enter a name, formula or CAS registry number or draw your compound. In the results, look for a link to an *interactive table*.

The screenshot shows the 'Structure/Property Search' page of the CRC Handbook of Chemistry and Physics. The page features a search bar at the top right and a table of contents on the left. The main content area is divided into three sections: 'Structure/Property Search', 'Chemical Structure', and 'Chemical Properties'. The 'Chemical Properties' section contains a table with columns for Property, Comparison, Value, and Action.

Property	Comparison	Value	Action
Name of substance	Contains		AND • [X] [Delete]
Formula	Equals		AND • [X] [Delete]
CAS Registry No.	Equals		AND • [X] [Delete]
Molecular weight	=		AND • [X] [Delete]
Subst.	Contains		[X] [Delete]

Use Chemical Structure AND Chemical Properties

[Search](#) [Clear Search Text](#)

A CRCwebBASE Product
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Knovel Library

This enables you to search across a range of different reference books including *DIPPR*, *Knovel Critical Tables* and *Yaws' Handbook of Physical Properties for Hydrocarbons and Chemicals*. Use the 'data search' link next to the main search box. Data is often provided in a table which may allow you to plot a graph, where appropriate. Don't reference the Knovel Library: write down the details of the specific book that the data comes from.

The screenshot shows the Knovel Search interface. The search bar contains the query 'material_or_substance_name:isobutyl alc' and the 'GO' button is highlighted. Below the search bar, there are navigation options: 'Home', 'Search for [query]', and 'Search within these results'. The main content area displays two search results under the heading 'INTERACTIVE TABLES'. The first result is 'Physical Properties of Organic Compounds (C-Table)' with 2 hits. It includes a table with columns: '#', 'index no.', 'material or substance name', 'synonyms', 'mol. formula', 'common formula', and 'CAS Regi'. The first row shows '814' and a link to 'CLICK LINK TO VIEW THE TABLE'. Below the table, it mentions 'from International Critical Tables of Numerical Data, Physics, Chemistry and Technology (1st Electronic Edition) (1926)'. The second result is 'Physical and Environmental Data of Chemical Compounds' with 1 hit. It includes a table with columns: '#', 'material or substance name', 'synonyms', 'mol. formula', 'CAS Registry No.', 'DOT no.', and 'mol. weig'. The first row shows '600' and a link to 'CLICK LINK TO VIEW THE TABLE'.

NIST Chemistry WebBook

Free, open access resource made available by the National Institute of Standards and Technology (USA). Search by compound name, CAS registry number, molecular formula or structure. The Chemistry WebBook is particularly useful for thermochemical data for both vapour and liquid phases, including enthalpy/entropy of formation, sublimation and fusion. Also provides Henry's Law data and ionisation energies. Melting and boiling points are available under 'phase change data': boiling point is labelled T_{boil} and melting point is labelled T_{fus} .

Condensed phase thermochemistry data

Go To: [Top](#), [References](#), [Notes](#) / [Error Report](#)

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Data compiled as indicated in comments:
ALS - H.Y. Afeefy, J.F. Liebman, and S.E. Stein
DH - E.S. Domalski and E.D. Hearing

Quantity	Value	Units	Method	Reference	Comment
$\Delta_f H^\circ_{\text{solid}}$	-165.0	kJ/mol	Ccb	Cox, 1961	ALS
$\Delta_f H^\circ_{\text{solid}}$	-165.1 ± 1.3	kJ/mol	Ccb	Andon, Biddiscombe, et al., 1960	ALS
$\Delta_f H^\circ_{\text{solid}}$	-162.8 ± 1.0	kJ/mol	Ccb	Parks, Manchester, et al., 1954	ALS
$\Delta_f H^\circ_{\text{solid}}$	-163.9	kJ/mol	Ccb	Badoche, 1941	Author's hf298_condensed=-41.49 kcal/mol; ALS
Quantity	Value	Units	Method	Reference	Comment
$\Delta_c H^\circ_{\text{solid}}$	-3058. ± 10.	kJ/mol	AVG	N/A	Average of 6 values; Individual data points
Quantity	Value	Units	Method	Reference	Comment
$S^\circ_{\text{solid}, 1 \text{ bar}}$	144.01	J/mol*K	N/A	Andon, Counsell, et al., 1963	DH
$S^\circ_{\text{solid}, 1 \text{ bar}}$	142.7	J/mol*K	N/A	Parks, Huffman, et al., 1933	Extrapolation below 90 K, 49.04 J/mol*K.; DH

ACD/i-Lab

Available via RSC National Chemical Database Service. This is primarily a tool for predicting properties but contains literature values for logP, solubility and pKa. Look for a link in the left hand menu that says 'DB'. DB means 'database' and gives experimental values.

Modules < **LogP DB Query setup (v12.1.0.50374)**

Phys Chem
- Absolv
- Basic PhysChem Properties (Free)
- Boiling Point/Vapor Pressure
- Adsorption Coefficient/BCF
- LogP
- LogD
- ACD pKa
- pKa
- Solubility
- Qualitative Solubility
- LogS
- **LogP DB**
- Solubility DB
- pKa DB
NMR
Naming

Structure
 Similar Structure
 SubStructure
 Exact Structure
 None

Common
Molecular Formula
Molecular Weight
LogP values
Reference
Name

Search by:

Search results of LogP DB

1 of 1

1. C₈H₉NO₂
4-Hydroxyacetanilide

Formula: C₈H₉NO₂
Compound Name: 4-Hydroxyacetanilide
Molecular Weight: 151.1626

[1] LogP: 0.250
Norrington, F.; Hyde, R.; Williams, S.; Wootton, F

[2] LogP: 0.360
Umeyama, H.; Nagai, T.; Nogami, H. Chem. Pharm. Bu

[3] LogP: 0.800 (Measured at pH = 7.2, phosphate
Hansch, C.; Leo, A.J. Substituent Constants for Cor

[4] LogP: 0.510 (presented in BioByte Star List)
La Rotonda, M.I.; Amato, G.; Barbato, F.; Silipo, C.;

[Download Report](#)

Detherm

Available via RSC National Chemical Database Service. Detherm gives thermophysical properties of pure substances **and mixtures** including vapour pressure, viscosity and phase equilibria.

SciFinder and Reaxys

These large literature databases provide property data for millions of compounds. They are best used to find data for compounds that are rarely reported in the literature: you will get too many values for common compounds and the values will vary considerably making it difficult to choose the 'correct' value. Property data is mainly derived from the journals and patents indexed by the databases: it is advisable to read the original article to view the conditions under which the data was obtained. SciFinder has additional data from a number of sources including graphical spectra from Wiley and AIST and predicted property values from ACDLabs.

For help with finding physical and chemical property data, please contact your subject librarian.