

Aspirin

Other names:

2-(Acetyloxy)benzoic acid
2-Acetoxybenzoic acid
2-Acetylsalicylic acid
2-Carboxyphenyl acetate
A.S.A.
A.S.A. Empirin
AC 5230
ASA
Acenterine
Acesal
Acesan
Acetal
Acetard
Aceticyl
Acetilsalicilico
Acetilum Acidulatum
Acetisal
Acetol
Acetonyl
Acetophen
Acetosal
Acetosalic acid
Acetosalin
Acetylin
Acetylsal
Acetylsalicylic acid
Acetylsalicylsaure
Acide acetylsalicylique
Acido O-acetil-benzoico
Acido acetilsalicilico
Acidum acetylsalicylicum
Acimetten
Acisal
Acylpyrin
Adiro
Asagran
Asatard
Ascoden-30
Ascolong
Aspalon

Aspec
Aspergum
Aspirdrops
Aspirine
Aspro
Asropharm
Asteric
Bayer
Benaspir
Benzoic acid, 2-(acetyloxy)-
Bi-prin
Bialpirina
Bialpirinia
Bufferin
Caprin
Cemirit
Claradin
Clariprin
Colfarit
Colsprin
Contrheuma retard
Coricidin
Crystar
Decaten
Delgesic
Dolean PH 8
Duramax
ECM
Easprin
Ecolen
Ecotrin
Empirin
Endydol
Entericin
Enterophen
Enterosarein
Enterosarine
Entrophen
Extren
Globentyl
Globoid
Helicon
Idragin

Kapsazal
Kyselina 2-acetoxybenzoova
Kyselina acetylsalicylova
Levius
Magnecyl
Measurin
Micristin
Miniasal
Neuronika
Novid
Nu-seals
Nu-seals aspirin
O-acetylsalicylic acid
Persistin
Pharmacin
Pirseal
Polopiryna
Premaspin
Rheumintabletten
Rhodine
Rhonal
S-211
SP 189
Salacetin
Salcetogen
Saletin
Salicylic acid acetate
Salicylic acid, acetyl-
Salicylacetylsalicylic acid
Solfrin
Solprin acid
Solpyron
Spira-Dine
St. Joseph
St. Joseph Aspirin for Adults
Supac
Tasprin
Temperal
Triaminicin
Triple-Sal
Xaxa
Yasta
Zorprin

benzoic acid, 2-acetoxy-
o-(Acetyloxy)benzoic acid
o-Acetoxybenzoic acid
o-Carboxyphenyl acetate

Inchi: InChI=1S/C9H8O4/c1-6(10)13-8-5-3-2-4-7(8)9(11)12/h2-5H,1H3,(H,11,12)
InchiKey: BSYNRYMUTXBXSQ-UHFFFAOYSA-N
Formula: C9H8O4
SMILES: CC(=O)Oc1ccccc1C(=O)O
Mol. weight [g/mol]: 180.16
CAS: 50-78-2

Physical Properties

Property code	Value	Unit	Source
gf	-371.98	kJ/mol	Joback Method
hf	-513.64	kJ/mol	Joback Method
hfus	33.85	kJ/mol	Thermodynamic properties of sublimation of the ortho and meta isomers of acetoxy and acetamido benzoic acids
hvap	71.15	kJ/mol	Joback Method
log10ws	-1.73		Aqueous and cosolvent solubility data for drug-like organic compounds
log10ws	-1.67		Aqueous Solubility Prediction Method
logp	1.310		Crippen Method
mvol	128.790	ml/mol	McGowan Method
pc	4082.92	kPa	Joback Method
rinpol	1309.00		NIST Webbook
rinpol	1270.00		NIST Webbook
rinpol	1315.00		NIST Webbook
rinpol	1309.00		NIST Webbook
rinpol	1270.00		NIST Webbook
tb	659.32	K	Joback Method
tc	868.49	K	Joback Method
tf	415.00 ± 3.00	K	NIST Webbook
tf	414.00 ± 5.00	K	NIST Webbook
tf	410.00 ± 6.00	K	NIST Webbook
tf	410.00 ± 5.00	K	NIST Webbook
tf	402.00 ± 10.00	K	NIST Webbook
tf	405.00 ± 10.00	K	NIST Webbook

tf	388.00 ± 15.00	K	NIST Webbook
tf	388.00 ± 15.00	K	NIST Webbook
tf	387.00 ± 15.00	K	NIST Webbook
tf	409.80 ± 4.00	K	NIST Webbook
tf	408.00 ± 5.00	K	NIST Webbook
tf	406.00 ± 5.00	K	NIST Webbook
tf	402.00 ± 6.00	K	NIST Webbook
tf	401.00 ± 6.00	K	NIST Webbook
tf	396.00 ± 8.00	K	NIST Webbook
tf	387.00 ± 8.00	K	NIST Webbook
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tf	388.00 ± 8.00	K	NIST Webbook
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tf	394.00 ± 6.00	K	NIST Webbook
tf	392.00 ± 6.00	K	NIST Webbook
tf	373.00 ± 6.00	K	NIST Webbook
tf	391.00 ± 6.00	K	NIST Webbook
tf	373.00 ± 6.00	K	NIST Webbook
tf	381.00 ± 10.00	K	NIST Webbook
tf	383.00 ± 10.00	K	NIST Webbook
tf	416.00 ± 3.00	K	NIST Webbook
tf	400.00 ± 2.00	K	NIST Webbook
tf	395.00 ± 2.00	K	NIST Webbook
tf	391.00 ± 2.00	K	NIST Webbook
tf	408.00 ± 5.00	K	NIST Webbook
tf	416.00 ± 3.00	K	NIST Webbook
tf	406.00 ± 10.00	K	NIST Webbook
tf	404.90 ± 2.00	K	NIST Webbook
tf	404.50 ± 2.00	K	NIST Webbook
tf	407.10 ± 2.50	K	NIST Webbook
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tf	408.00 ± 1.50	K	NIST Webbook
tf	407.40 ± 0.50	K	NIST Webbook
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tf	134.80 ± 0.50	K	NIST Webbook
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tf	405.20 ± 2.00	K	NIST Webbook
tf	273.15 ± 5.00	K	NIST Webbook
tf	405.00 ± 3.00	K	NIST Webbook
tf	398.00 ± 6.00	K	NIST Webbook
tf	397.70 ± 3.00	K	NIST Webbook
tf	510.00 ± 4.00	K	NIST Webbook
tf	412.00 ± 5.00	K	NIST Webbook
tf	405.00 ± 12.00	K	NIST Webbook
tf	414.00 ± 4.00	K	NIST Webbook
tf	409.00 ± 3.00	K	NIST Webbook
tf	408.50	K	Polar Mixed-Solid Solute Systems in Supercritical Carbon Dioxide: Entrainer Effect and Its Influence on Solubility and Selectivity
tf	408.15	K	Liquid pharmaceuticals formulation by eutectic formation
tf	408.65	K	Determination and prediction of solubilities of active pharmaceutical ingredients in selected organic solvents
tf	410.19	K	Aqueous Solubility Prediction Method
tf	407.90 ± 2.00	K	NIST Webbook
vc	0.480	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	346.00	J/mol×K	798.77	Joback Method
cpg	358.88	J/mol×K	868.49	Joback Method
cpg	352.72	J/mol×K	833.63	Joback Method
cpg	313.39	J/mol×K	659.32	Joback Method
cpg	322.42	J/mol×K	694.18	Joback Method
cpg	330.85	J/mol×K	729.04	Joback Method
cpg	338.71	J/mol×K	763.90	Joback Method
dvisc	0.0000688	Paxs	659.32	Joback Method
dvisc	0.0001455	Paxs	577.23	Joback Method

dvisc	0.0000976	Paxs	618.27	Joback Method
dvisc	0.0015914	Paxs	413.04	Joback Method
dvisc	0.0007440	Paxs	454.09	Joback Method
dvisc	0.0003946	Paxs	495.13	Joback Method
dvisc	0.0002306	Paxs	536.18	Joback Method
hfust	29.80	kJ/mol	414.00	NIST Webbook
hfust	31.01	kJ/mol	412.70	NIST Webbook
hfust	29.17	kJ/mol	409.20	NIST Webbook

Sources

Apparent Molal Volumes and Viscosity B-Coefficients of Acetyl Salicylic Acid in Pure Solvents Using Focus-Induced Beam Refraction Measurements	https://www.doi.org/10.1021/je9004646
Solubility of Benzoin Acid and Aspirin in Supercritical CO ₂ with and without Ethanol	https://www.doi.org/10.1021/acs.jced.5b00746
Supercritical CO ₂ Solubility of Ketoprofen and Aspirin in Supercritical CO ₂ by Liquid-Space-Trap's formulation by eutectic formation: Density, Viscosity, Speed of Sound, and Refractive Index of a Ternary System	https://www.doi.org/10.1021/acs.jced.5b00812
Supercritical CO ₂ Solubility of Ketoprofen and Aspirin in Supercritical CO ₂ by Liquid-Space-Trap's formulation by eutectic formation: Density, Viscosity, Speed of Sound, and Refractive Index of a Ternary System	https://www.doi.org/10.1016/j.fluid.2017.05.009
Supercritical CO ₂ Solubility of Ketoprofen and Aspirin in Supercritical CO ₂ by Liquid-Space-Trap's formulation by eutectic formation: Density, Viscosity, Speed of Sound, and Refractive Index of a Ternary System	https://www.doi.org/10.1021/je5008372
Supercritical CO ₂ Solubility of Ketoprofen and Aspirin in Supercritical CO ₂ by Liquid-Space-Trap's formulation by eutectic formation: Density, Viscosity, Speed of Sound, and Refractive Index of a Ternary System	http://pubs.acs.org/doi/abs/10.1021/ci9903071
1-Butyl-3-methylimidazolium Bromide, Aqueous Solubility Prediction Method: Temperatures T = (288.15 to 318.15) K: Joback Method	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDataset002.xlsx
NIST Webbook:	https://en.wikipedia.org/wiki/Joback_method
Determination and prediction of solubilities of active pharmaceutical ingredients in cosolvent systems: Aqueous and cosolvent solubility data for drug-like organic compounds: Polar Mixed-Solid Solute Systems in Supercritical Carbon Dioxide: Entrainer Effect of aspirin in supercritical carbon dioxide/alcohol mixtures: Thermodynamic properties of sublimation of the ortho and meta isomers of acetylsalicylic acid in Ethanol, Acetone, Propylene Glycol, and 2-Propanol	http://webbook.nist.gov/cgi/cbook.cgi?ID=C50782&Units=SI
	https://www.doi.org/10.1016/j.fluid.2015.07.032
	https://www.ncbi.nlm.nih.gov/pmc/articles/PMC2751500/
	https://www.doi.org/10.1021/je700486g
	https://www.doi.org/10.1016/j.fluid.2005.08.004
	https://www.doi.org/10.1016/j.jct.2015.02.010
	https://www.doi.org/10.1021/je7005693
	http://link.springer.com/article/10.1007/BF02311772
Solubility of Aspirin in Supercritical Carbon Dioxide with and without Acetone:	https://www.doi.org/10.1021/je0499465

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hfust:	Enthalpy of fusion at a given temperature
hvap:	Enthalpy of vaporization at standard conditions

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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