Aspirin

Other names:

2-(Acetyloxy)benzoic acid
2-Acetoxybenzoic acid
2-Acetylsalicyclic 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
Aspropharm
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-
Salycylacetylsalicylic 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	33.51 ± 0.04	kJ/mol	Determination and prediction of solubilities of active pharmaceutical ingredients in selected organic solvents
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
mcvol	128.790	ml/mol	McGowan Method
pc	4082.92	kPa	Joback Method
rinpol	1315.00		NIST Webbook
rinpol	1309.00		NIST Webbook
rinpol	1270.00		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	407.50 ± 2.00	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
tf	397.00 ± 8.00	K	NIST Webbook
tf	388.00 ± 8.00	K	NIST Webbook
tf	396.00 ± 6.00	K	NIST Webbook
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
tf	406.40 ± 2.00	K	NIST Webbook
tf	407.80 ± 2.00	K	NIST Webbook
tf	407.00 ± 2.50	K	NIST Webbook
tf	404.50 ± 2.00	K	NIST Webbook
tf	404.30 ± 2.00	K	NIST Webbook
tf	405.80 ± 2.00	K	NIST Webbook
tf	405.30 ± 2.00	K	NIST Webbook
tf	409.00 ± 2.50	K	NIST Webbook
tf	407.30 ± 2.00	K	NIST Webbook
tf	405.25 ± 2.00	K	NIST Webbook
tf	403.50 ± 2.00	K	NIST Webbook
tf	406.80 ± 2.00	K	NIST Webbook
tf	405.90 ± 2.00	K	NIST Webbook
tf	409.30 ± 2.00	K	NIST Webbook
tf	407.10 ± 2.00	K	NIST Webbook
tf	404.70 ± 2.00	K	NIST Webbook
tf	404.80 ± 2.00	K	NIST Webbook
tf	406.50 ± 2.00	K	NIST Webbook

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tf	388.00 ± 15.00	K	NIST Webbook
tf	404.10 ± 2.00	K	NIST Webbook
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tf	407.20 ± 2.50	K	NIST Webbook
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tf	406.30 ± 2.00	K	NIST Webbook
tf	407.60 ± 2.00	K	NIST Webbook
tf	407.20 ± 2.00	K	NIST Webbook
tf	402.20 ± 4.00	K	NIST Webbook
tf	406.70 ± 2.00	K	NIST Webbook
tf	406.20 ± 2.00	K	NIST Webbook
tf	407.20 ± 2.00	K	NIST Webbook
tf	407.20 ± 2.00	K	NIST Webbook
tf	407.70 ± 2.00	K	NIST Webbook
tf	408.00 ± 2.00	K	NIST Webbook
tf	406.20 ± 2.00	K	NIST Webbook
tf	409.00 ± 2.00	K	NIST Webbook
tf	408.20 ± 2.00	K	NIST Webbook
tf	406.80 ± 0.50	K	NIST Webbook
tf	406.80 ± 0.50	K	NIST Webbook
tf	406.60 ± 0.50	K	NIST Webbook
tf	407.80 ± 2.00	K	NIST Webbook
tf	402.10 ± 4.00	K	NIST Webbook
tf	402.50 ± 4.00	K	NIST Webbook
tf	405.90 ± 3.00	K	NIST Webbook
tf	406.90 ± 3.00	K	NIST Webbook
tf	407.00 ± 3.00	K	NIST Webbook
tf	408.00 ± 1.50	K	NIST Webbook
tf	407.40 ± 0.50	K	NIST Webbook
tf	407.70 ± 0.50	K	NIST Webbook
tf	134.80 ± 0.50	K	NIST Webbook
tf	407.00 ± 3.00	K	NIST Webbook
tf	412.00 ± 4.00	K	NIST Webbook
tf	407.20 ± 2.00	K	NIST Webbook
tf	407.20 ± 2.00	K	NIST Webbook
tf	407.10 ± 3.00	K	NIST Webbook
tf	407.50 ± 2.00	K	NIST Webbook
tf	405.40 ± 1.00	K	NIST Webbook
tf	407.90 ± 2.00	K	NIST Webbook
tf	405.40 ± 1.00	K	NIST Webbook
tf	407.90 ± 2.00	K	NIST Webbook
tf	405.40 ± 1.00	K	NIST Webbook

tf	407.90 ± 2.00	K	NIST Webbook
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	388.00 ± 15.00	K	NIST Webbook
tf	405.00 ± 10.00	K	NIST Webbook
tf	402.00 ± 10.00	K	NIST Webbook
tf	410.00 ± 5.00	K	NIST Webbook
tf	410.00 ± 6.00	K	NIST Webbook
tf	414.00 ± 5.00	K	NIST Webbook
tf	415.00 ± 3.00	K	NIST Webbook
tf	403.00 ± 8.00	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	408.65 ± 0.30	K	Determination and prediction of solubilities of active pharmaceutical ingredients in selected organic solvents
tf	407.38	K	Thermodynamic properties of sublimation of the ortho and meta isomers of acetoxy and acetamido benzoic acids
tf	408.15	K	Liquid pharmaceuticals formulation by eutectic formation
tf	410.19	K	Aqueous Solubility Prediction Method
vc	0.480	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
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
cpg	346.00	J/mol×K	798.77	Joback Method
cpg	352.72	J/mol×K	833.63	Joback Method
cpg	358.88	J/mol×K	868.49	Joback Method
cps	239.00	J/mol×K	298.00	Liquid pharmaceuticals formulation by eutectic formation
dvisc	0.0007440	Pa×s	454.09	Joback Method
dvisc	0.0015914	Pa×s	413.04	Joback Method
dvisc	0.0003946	Pa×s	495.13	Joback Method
dvisc	0.0002306	Pa×s	536.18	Joback Method
dvisc	0.0001455	Pa×s	577.23	Joback Method
dvisc	0.0000976	Pa×s	618.27	Joback Method
dvisc	0.0000688	Pa×s	659.32	Joback Method
hfust	29.17	kJ/mol	409.20	NIST Webbook
hfust	31.01	kJ/mol	412.70	NIST Webbook
hfust	29.80	kJ/mol	414.00	NIST Webbook
psub	2.03e-04	kPa	345.28	Thermodynamic properties of sublimation of the ortho and meta isomers of acetoxy and acetamido benzoic acids
psub	1.58e-04	kPa	343.24	Thermodynamic properties of sublimation of the ortho and meta isomers of acetoxy and acetamido benzoic acids
psub	1.20e-04	kPa	341.11	Thermodynamic properties of sublimation of the ortho and meta isomers of acetoxy and acetamido benzoic acids
psub	2.38e-04	kPa	347.10	Thermodynamic properties of sublimation of the ortho and meta isomers of acetoxy and acetamido benzoic acids

psub	3.05e-04	kPa	349.24	Thermodynamic properties of sublimation of the ortho and meta isomers of acetoxy and acetamido benzoic acids	
psub	3.87e-04	kPa	351.27	Thermodynamic properties of sublimation of the ortho and meta isomers of acetoxy and acetamido benzoic acids	
psub	4.71e-04	kPa	353.10	Thermodynamic properties of sublimation of the ortho and meta isomers of acetoxy and acetamido benzoic acids	
psub	6.43e-04	kPa	355.28	Thermodynamic properties of sublimation of the ortho and meta isomers of acetoxy and acetamido benzoic acids	
psub	7.96e-04	kPa	357.27	Thermodynamic properties of sublimation of the ortho and meta isomers of acetoxy and acetamido benzoic acids	
psub	9.66e-04	kPa	359.23	Thermodynamic properties of sublimation of the ortho and meta isomers of acetoxy and acetamido benzoic acids	
psub	1.17e-03	kPa	361.11	Thermodynamic properties of sublimation of the ortho and meta isomers of acetoxy and acetamido benzoic acids	

psub	1.19e-04	kPa	341.11	Thermodynamic properties of sublimation of the ortho and meta isomers of acetoxy and acetamido benzoic acids	
psub	1.47e-04	kPa	343.24	Thermodynamic properties of sublimation of the ortho and meta isomers of acetoxy and acetamido benzoic acids	
psub	1.94e-04	kPa	345.28	Thermodynamic properties of sublimation of the ortho and meta isomers of acetoxy and acetamido benzoic acids	
psub	2.30e-04	kPa	347.10	Thermodynamic properties of sublimation of the ortho and meta isomers of acetoxy and acetamido benzoic acids	
psub	2.90e-04	kPa	349.24	Thermodynamic properties of sublimation of the ortho and meta isomers of acetoxy and acetamido benzoic acids	
psub	3.78e-04	kPa	351.27	Thermodynamic properties of sublimation of the ortho and meta isomers of acetoxy and acetamido benzoic acids	
psub	4.78e-04	kPa	353.10	Thermodynamic properties of sublimation of the ortho and meta isomers of acetoxy and acetamido benzoic acids	

psub	5.99e-04	kPa	355.28	Thermodynamic properties of sublimation of the ortho and meta isomers of acetoxy and acetamido benzoic acids
psub	7.44e-04	kPa	357.27	Thermodynamic properties of sublimation of the ortho and meta isomers of acetoxy and acetamido benzoic acids
psub	8.90e-04	kPa	359.23	Thermodynamic properties of sublimation of the ortho and meta isomers of acetoxy and acetamido benzoic acids
psub	1.17e-03	kPa	361.11	Thermodynamic properties of sublimation of the ortho and meta isomers of acetoxy and acetamido benzoic acids

Sources

Polar Mixed-Solid Solute Systems in Supercritical Carbon Dioxide: Entrainer Effect and Its Influence on Solubility and Selectivity:	https://www.doi.org/10.1021/je700486g
Aqueous and cosolvent solubility data for drug-like organic compounds:	https://www.ncbi.nlm.nih.gov/pmc/articles/PMC2751500/
Liquid pharmaceuticals formulation by eutectic formation:	https://www.doi.org/10.1016/j.fluid.2017.05.009
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Thermodynamic properties of sublimation of the ortho and meta isomers of acetoxy and acetamido benzoic acids:	https://www.doi.org/10.1016/j.jct.2015.02.010
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
Determination and prediction of solubilities of active pharmaceutical ingredients in selected organic solvents:	https://www.doi.org/10.1016/j.fluid.2015.07.032
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C50782&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

cpg:	Ideal gas heat capacity
cps:	Solid phase 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
psub:	Sublimation pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume