

Vanillic acid

Other names:	3-Methoxy-4-Hydroxybenzoic acid
	4-Hydroxy-3-methoxybenzoic acid
	4-Hydroxy-3-methoxybenzoic acid (vanillic acid)
	Acide vanillique
	Benzoic acid, 4-hydroxy-3-methoxy-
	NSC 3987
	NSC 674322
	Protocatechuic acid, 3-methyl ester
	VA
	m-Anisic acid, 4-hydroxy-
Inchi:	InChI=1S/C8H8O4/c1-12-7-4-5(8(10)11)2-3-6(7)9/h2-4,9H,1H3,(H,10,11)
InchiKey:	WKOLLVMJNQIZCI-UHFFFAOYSA-N
Formula:	C8H8O4
SMILES:	COc1cc(C(=O)O)ccc1O
Mol. weight [g/mol]:	168.15
CAS:	121-34-6

Physical Properties

Property code	Value	Unit	Source
gf	-406.10	kJ/mol	Joback Method
hf	-557.73	kJ/mol	Joback Method
hfus	22.79	kJ/mol	Joback Method
hvap	75.19	kJ/mol	Joback Method
log10ws	-2.05		Aqueous Solubility Prediction Method
logp	1.099		Crippen Method
mcvol	119.000	ml/mol	McGowan Method
pc	5228.24	kPa	Joback Method
rinpol	1620.00		NIST Webbook
rinpol	1570.00		NIST Webbook
rinpol	1608.00		NIST Webbook
rinpol	1566.00		NIST Webbook
rinpol	1592.00		NIST Webbook
rinpol	1566.00		NIST Webbook
tb	663.19	K	Joback Method
tc	878.05	K	Joback Method

tf	484.90	K	Measurement and Correlation of the Solubility of Vanillic Acid in Eight Pure and Water + Ethanol Mixed Solvents at Temperatures from (293.15 to 323.15) K
tf	483.00 ± 5.00	K	NIST Webbook
tf	478.00 ± 4.00	K	NIST Webbook
tf	480.70	K	Solubility of high-value compounds in ethyl lactate: Measurements and modelling
tf	485.48	K	Aqueous Solubility Prediction Method
vc	0.385	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	298.09	J/mol×K	663.19	Joback Method
cpg	306.15	J/mol×K	699.00	Joback Method
cpg	313.72	J/mol×K	734.81	Joback Method
cpg	320.86	J/mol×K	770.62	Joback Method
cpg	327.60	J/mol×K	806.43	Joback Method
cpg	333.98	J/mol×K	842.24	Joback Method
cpg	340.07	J/mol×K	878.05	Joback Method
dvisc	0.0003059	Pa×s	463.56	Joback Method
dvisc	0.0001353	Pa×s	496.83	Joback Method
dvisc	0.0000663	Pa×s	530.10	Joback Method
dvisc	0.0000353	Pa×s	563.38	Joback Method
dvisc	0.0000202	Pa×s	596.65	Joback Method
dvisc	0.0000123	Pa×s	629.92	Joback Method
dvisc	0.0000078	Pa×s	663.19	Joback Method

Sources

Solubility of high-value compounds in ethyl lactate: Measurements and Correlation Method: <https://www.doi.org/10.1016/j.jct.2011.12.005>
<http://pubs.acs.org/doi/abs/10.1021/ci990307l>

Solubility of Syringic and Vanillic Acids in Supercritical Carbon Dioxide: <https://www.doi.org/10.1021/je034129a>

Solubility of high-value compounds in environmentally friendly solvents liquid <https://www.doi.org/10.1016/j.jct.2013.10.036>

Solubility of Syringic and Vanillic Acids in Supercritical Carbon Dioxide: <https://www.doi.org/10.1021/acs.jced.6b00322>

Solubility of Syringic and Vanillic Acids in Supercritical Carbon Dioxide: <https://www.doi.org/10.1021/acs.jced.6b00322>

Aqueous Solubility Prediction Method: <http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDataset002.xlsx>

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>

Temperature and salt addition effects on the solubility behaviour of some phenolic compounds in water: <https://www.doi.org/10.1016/j.jct.2006.06.014>

Solubility of some phenolic compounds in aqueous alkali metal methoxide and correlation of the 15 <https://www.doi.org/10.1016/j.jct.2008.06.006>

Measurement and Correlation of the Solubility of Vanillic Acid in Eight Pure and Water and Ethanol Mixed Solvents at <https://www.doi.org/10.1021/acs.jced.5b00619>

Behavior of Syringic Acid in Eight Pure and Water and Methanol Mixed Solvents: <https://www.doi.org/10.1021/acs.jced.7b00333>

Joback Method: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C121346&Units=SI>

https://en.wikipedia.org/wiki/Joback_method

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
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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