p-Coumaric acid

Other names:	.beta.-(4-hydroxyphenyl)acrylic acid
	2-propenoic acid, 3-(4-hydroxyphenyl)-
	3-(4-hydroxyphenyl)-2-propenoic acid
	4'-Hydroxycinnamic acid
	4-coumaric acid
	4-hydroxycinnamic acid
	Cinnamic acid, p-hydroxy-
	NSC 59260
	p-Cumaric acid
	p-Hydroxyphenylacrylic acid
	p-hydroxycinnamic acid
	para-Coumaric acid
	«beta»-(4-Hydroxyphenyl)acrylic acid
Inchi:	InChI=1S/C9H8O3/c10-8-4-1-7(2-5-8)3-6-9(11)12/h1-6,10H,(H,11,12)/b6-3+
InchiKey:	NGSWKAQJJWESNS-ZZXKWVIFSA-N
Formula:	C9H8O3
SMILES:	O=C(O)C=Cc1ccc(O)cc1
Mol. weight [g/mol]:	164.16
CAS:	7400-08-0

Physical Properties

Property code	Value	Unit	Source
gf	-202.83	kJ/mol	Joback Method
hf	-317.46	kJ/mol	Joback Method
hfus	24.78	kJ/mol	Joback Method
hvap	74.30	kJ/mol	Joback Method
log10ws	-1.36		Crippen Method
logp	1.490		Crippen Method
mcvol	122.920	ml/mol	McGowan Method
pc	5138.68	kPa	Joback Method
rinpol	1635.00		NIST Webbook
rinpol	1631.00		NIST Webbook
tb	662.83	K	Joback Method
tc	884.22	K	Joback Method
tf	489.00 ± 5.00	K	NIST Webbook
tf	486.90 ± 3.00	K	NIST Webbook
tf	475.00 ± 5.00	K	NIST Webbook

tf	494.30	K	Measurement and Correlation of the Solubility of p-Coumaric Acid in Nine Pure and Water + Ethanol Mixed Solvents at Temperatures from 293.15 to 333.15 K
tf	492.35	K	Solubilities of p-coumaric and caffeic acid in ionic liquids and organic solvents
vc	0.403	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	302.19	J/mol×K	662.83	Joback Method
cpg	310.51	J/mol×K	699.73	Joback Method
cpg	318.25	J/mol×K	736.63	Joback Method
cpg	325.49	J/mol×K	773.52	Joback Method
cpg	332.34	J/mol×K	810.42	Joback Method
cpg	338.88	J/mol×K	847.32	Joback Method
cpg	345.20	J/mol×K	884.22	Joback Method
dvisc	0.0006684	Pa×s	435.00	Joback Method
dvisc	0.0002358	Pa×s	472.97	Joback Method
dvisc	0.0000971	Pa×s	510.94	Joback Method
dvisc	0.0000452	Pa×s	548.91	Joback Method
dvisc	0.0000232	Pa×s	586.89	Joback Method
dvisc	0.0000130	Pa×s	624.86	Joback Method
dvisc	0.0000077	Pa×s	662.83	Joback Method

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C7400080&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Solubilities of p-coumaric and caffeic acid in ionic liquids and organic solvents:	https://www.doi.org/10.1016/j.jct.2013.02.013
Measurement and Correlation of the Solubility of p-Coumaric Acid in Nine Pure and Water + Ethanol Mixed Solvents at Temperatures from 293.15 to 333.15 K:	https://www.doi.org/10.1021/acs.jced.6b00361
Determination and Thermodynamic Modeling of Solid-Liquid Phase Equilibrium for Esomeprazole Sodium in Monosolvents and in the (Ethanol + Ethyl Acetate) Binary Solvent Mixtures:	https://www.doi.org/10.1021/acs.jced.6b01044

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