Caffeic acid

Other names:	2-Propenoic acid, 3-(3,4-dihydroxyphenyl)-
	Cinnamic acid, 3,4-dihydroxy-
	3-(3,4-Dihydroxyphenyl)-2-propenoic acid
	3-(3,4-Dihydroxyphenyl)propenoic acid
	3,4-Dihydroxybenzeneacrylic acid
	3,4-Dihydroxycinnamic acid
	4-(2-Carboxyethenyl)-1,2-dihydroxybenzene
	4-(2'-Carboxyvinyl)-1,2-dihydroxybenzene
	NSC 57197
	3,4-Dihydroxycinnamic acid (caffeic acid)
Inchi:	InChI=1S/C9H8O4/c10-7-3-1-6(5-8(7)11)2-4-9(12)13/h1-5,10-11H,(H,12,13)/b4-2+
InchiKey:	QAIPRVGONGVQAS-DUXPYHPUSA-N
Formula:	C9H8O4
SMILES:	O=C(O)C=Cc1ccc(O)c(O)c1
Mol. weight [g/mol]:	180.16
CAS:	331-39-5

Physical Properties

Property code	Value	Unit	Source
gf	-357.45	kJ/mol	Joback Method
hf	-494.77	kJ/mol	Joback Method
hfus	30.56	kJ/mol	Joback Method
hvap	87.31	kJ/mol	Joback Method
log10ws	-0.91		Crippen Method
logp	1.196		Crippen Method
mcvol	128.790	ml/mol	McGowan Method
pc	6441.16	kPa	Joback Method
rinpol	1478.00		NIST Webbook
tb	743.45	K	Joback Method
tc	972.70	K	Joback Method
tf	546.72	K	Joback Method
vc	0.368	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	381.42	J/mol×K	972.70	Joback Method
cpg	373.93	J/mol×K	934.49	Joback Method
cpg	366.78	J/mol×K	896.28	Joback Method
cpg	359.81	J/mol×K	858.07	Joback Method
cpg	352.90	J/mol×K	819.87	Joback Method
cpg	345.89	J/mol×K	781.66	Joback Method
cpg	338.64	J/mol×K	743.45	Joback Method
dvisc	0.0000171	Pa×s	546.72	Joback Method
dvisc	0.0000003	Pa×s	743.45	Joback Method
dvisc	0.0000005	Pa×s	710.66	Joback Method
dvisc	0.0000010	Pa×s	677.87	Joback Method
dvisc	0.0000018	Pa×s	645.09	Joback Method
dvisc	0.0000035	Pa×s	612.30	Joback Method
dvisc	0.0000074	Pa×s	579.51	Joback Method
hsubt	170.20 ± 4.60	kJ/mol	416.50	NIST Webbook

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
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=C331395&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
hsubt: Enthalpy of sublimation 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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