Cinnamic acid, 3,4-dihydroxy-

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=C/c1ccc(O)c(O)c1
Mol. weight [g/mol]:	180.16

Physical Properties

Property code	Value	Unit	Source
hfus	30.56	kJ/mol	Joback Method
ie	8.21	eV	Cheméo Relay (1.0)
log10ws	-1.74		Cheméo Relay (1.0)
logp	1.196		Crippen Method
mcvol	128.790	ml/mol	McGowan Method
rinpol	1478.00		NIST Webbook
tb	599.71	K	Cheméo Relay (1.0)
tf	481.26	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	338.64	J/mol×K	743.45	Joback Method
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
dvisc	0.0000018	Pa×s	645.09	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	0.0000171	Pa×s	546.72	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
Cheméo Relay (1.0):
Cheméo Relay (1.0, beta):
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C331395&Units=SI
Joback Method: https://en.wikipedia.org/wiki/Joback_method
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

cpg: Ideal gas heat capacity
dvisc: Dynamic viscosity
hfus: Enthalpy of fusion at standard conditions
hsubt: Enthalpy of sublimation at a given temperature
ie: Ionization energy
log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
rinpol: Non-polar retention indices
tb: Normal Boiling Point Temperature
tf: Normal melting (fusion) point