3,4-Dimethoxycinnamic acid

Other names:	Dimethyl caffeic acid
	2-Propenoic acid, 3-(3,4-dimethoxyphenyl)-
	Caffeic acid dimethyl ether
	Cinnamic acid, 3,4-dimethoxy-
	3,4-Dimethoxyphenyl-2-propenoic acid
	3,4-Di-O-methylcaffeic acid
	Methylferulic acid
	O,O-Dimethylcaffeic acid
	o-Methylferulic acid
	NSC 4323
	NSC 43569
	trans-3,4-Dimethoxycinnamic acid
	(2E)-3-(3,4-Dimethoxyphenyl)-2-propenoic acid
Inchi:	InChI=1S/C11H12O4/c1-14-9-5-3-8(4-6-11(12)13)7-10(9)15-2/h3-7H,1-2H3,(H,12,13)/b6
InchiKey:	HJBWJAPEBGSQPR-GQCTYLIASA-N
Formula:	C11H12O4
SMILES:	COc1ccc(C=CC(=O)O)cc1OC
Mol. weight [g/mol]:	208.21
CAS:	2316-26-9

Physical Properties

Property code	Value	Unit	Source
gf	-260.63	kJ/mol	Joback Method
hf	-468.81	kJ/mol	Joback Method
hfus	25.77	kJ/mol	Joback Method
hsub	149.90 ± 0.80	kJ/mol	NIST Webbook
hvap	71.88	kJ/mol	Joback Method
log10ws	-2.05		Crippen Method
logp	1.802		Crippen Method
mcvol	156.970	ml/mol	McGowan Method
pc	3086.42	kPa	Joback Method
rinpol	1926.20		NIST Webbook
rinpol	1926.20		NIST Webbook
tb	682.77	K	Joback Method
tc	886.19	K	Joback Method
tf	415.32	K	Joback Method
vc	0.585	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	399.37	J/mol×K	682.77	Joback Method
cpg	410.13	J/mol×K	716.67	Joback Method
cpg	420.26	J/mol×K	750.58	Joback Method
cpg	429.78	J/mol×K	784.48	Joback Method
cpg	438.68	J/mol×K	818.39	Joback Method
cpg	446.99	J/mol×K	852.29	Joback Method
cpg	454.69	J/mol×K	886.19	Joback Method
dvisc	0.0009159	Pa×s	415.32	Joback Method
dvisc	0.0004082	Pa×s	459.89	Joback Method
dvisc	0.0002098	Pa×s	504.47	Joback Method
dvisc	0.0001202	Pa×s	549.04	Joback Method
dvisc	0.0000748	Pa×s	593.62	Joback Method
dvisc	0.0000498	Pa×s	638.19	Joback Method
dvisc	0.0000349	Pa×s	682.77	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C2316269&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method: 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
hsub: Enthalpy of sublimation 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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