3,5-Dimethoxycinnamic acid

Other names: 2-Propenoic acid, 3-(3,5-dimethoxyphenyl)-
Cinnamic acid, 3,5-dimethoxy-
3,5-Dimethoxycinnamic acid, predominantly trans
3',5'-dimethoxycinnamic acid
trans-3,5-dimethoxycinnamic acid
Inchi: InChI=1S/C11H12O4/c1-14-9-5-8(3-4-11(12)13)6-10(7-9)15-2/h3-7H,1-2H3,(H,12,13)/b4
InchiKey: VLSRUFWCGBMYDJ-ONEGZZNKSA-N
Formula: C11H12O4
SMILES: COc1cc(C=CC(=O)O)cc(OC)c1
Mol. weight [g/mol]: 208.21
CAS: 16909-11-8

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	141.40 ± 0.50	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	1918.30		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	446.99	J/mol×K	852.29	Joback Method

cpg	438.68	J/mol×K	818.39	Joback Method
cpg	429.78	J/mol×K	784.48	Joback Method
cpg	420.26	J/mol×K	750.58	Joback Method
cpg	410.13	J/mol×K	716.67	Joback Method
cpg	454.69	J/mol×K	886.19	Joback Method
dvisc	0.0000349	Pa×s	682.77	Joback Method
dvisc	0.0000498	Pa×s	638.19	Joback Method
dvisc	0.0000748	Pa×s	593.62	Joback Method
dvisc	0.0001202	Pa×s	549.04	Joback Method
dvisc	0.0002098	Pa×s	504.47	Joback Method
dvisc	0.0004082	Pa×s	459.89	Joback Method
dvisc	0.0009159	Pa×s	415.32	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C16909118&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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