2-Propenoic acid, 3-(3,4-dimethoxyphenyl)-, (E)-

Other names: (2E)-3-(3,4-Dimethoxyphenyl)-2-propenoic acid
(E)-3,4-Dimethoxycinnamic acid
(E)-3',4'-dimethoxycinnamic 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: 14737-89-4

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
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	1949.00		NIST Webbook
rinpol	1949.00		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

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C14737894&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
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

Latest version available from: