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

Other names: trans-2,3-Dimethoxycinnamic acid
(2E)-3-(2,3-Dimethoxyphenyl)-2-propenoic acid
Inchi: InChI=1S/C11H12O4/c1-14-9-5-3-4-8(11(9)15-2)6-7-10(12)13/h3-7H,1-2H3,(H,12,13)/b7
InchiKey: QAXPUWGAGVERSJ-VOTSOKGWSA-N
Formula: C11H12O4
SMILES: COc1cccc(C=CC(=O)O)c1OC
Mol. weight [g/mol]: 208.21
CAS: 7345-82-6

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	141.00 ± 0.90	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	1818.80		NIST Webbook
rinpol	1818.80		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

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=C7345826&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
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