2,3,4-Trimethoxycinnamic acid

Other names: 2-Propenoic acid, 3-(2,3,4-trimethoxyphenyl)-
trans-2,3,4-trimethoxycinnamic acid
Inchi: InChI=1S/C12H14O5/c1-15-9-6-4-8(5-7-10(13)14)11(16-2)12(9)17-3/h4-7H,1-3H3,(H,13,
InchiKey: ZYOPDNLIHHFGEC-FNORWQNLSA-N
Formula: C12H14O5
SMILES: COc1ccc(C=CC(=O)O)c(OC)c1OC
Mol. weight [g/mol]: 238.24
CAS: 33130-03-9

Physical Properties

Property code	Value	Unit	Source
gf	-366.84	kJ/mol	Joback Method
hf	-633.14	kJ/mol	Joback Method
hfus	29.16	kJ/mol	Joback Method
hvap	77.18	kJ/mol	Joback Method
log10ws	-2.17		Crippen Method
logp	1.810		Crippen Method
mcvol	176.930	ml/mol	McGowan Method
pc	2690.21	kPa	Joback Method
tb	733.05	K	Joback Method
tc	933.80	K	Joback Method
tf	461.34	K	Joback Method
vc	0.658	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	473.43	J/mol×K	733.05	Joback Method
cpg	484.59	J/mol×K	766.51	Joback Method
cpg	495.08	J/mol×K	799.97	Joback Method
cpg	504.89	J/mol×K	833.43	Joback Method
cpg	514.02	J/mol×K	866.89	Joback Method
cpg	522.45	J/mol×K	900.34	Joback Method
cpg	530.18	J/mol×K	933.80	Joback Method

dvisc	0.0003992	Pa×s	461.34	Joback Method
dvisc	0.0001976	Pa×s	506.62	Joback Method
dvisc	0.0001098	Pa×s	551.91	Joback Method
dvisc	0.0000667	Pa×s	597.19	Joback Method
dvisc	0.0000435	Pa×s	642.48	Joback Method
dvisc	0.0000300	Pa×s	687.76	Joback Method
dvisc	0.0000216	Pa×s	733.05	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=C33130039&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
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume