2-Propenoic acid, 3-(3,4-dimethoxyphenyl)-, methyl ester

Other names: Cinnamic acid, 3,4-dimethoxy-, methyl ester
Methyl 3,4-dimethoxycinnamate
3,4-O-Dimethylcaffeic acid methyl ester
Methyl ester of 3,4-Dimethoxycinnamic acid
3,4-Dimethoxy-trans-cinnamic acid,methyl ester
Methyl 3-(3,4-dimethoxyphenyl)-2-propenoate
Methyl 3-(3,4-dimethoxyphenyl)acrylate
Methyl 3-(3,4-dimethoxyphenyl)-prop-2-enoate
3,4-Dimethoxy methyl cinnamate

Inchi: InChI=1S/C12H14O4/c1-14-10-6-4-9(8-11(10)15-2)5-7-12(13)16-3/h4-8H,1-3H3/b7-5+

InchiKey: JXRYDOZRPYFBKO-FNORWQNLSA-N

Formula: C12H14O4

SMILES: COC(=O)C=Cc1ccc(OC)c(OC)c1

Mol. weight [g/mol]: 222.24

CAS: 5396-64-5

Physical Properties

Property code	Value	Unit	Source
gf	-220.39	kJ/mol	Joback Method
hf	-469.44	kJ/mol	Joback Method
hfus	25.46	kJ/mol	Joback Method
hvap	59.84	kJ/mol	Joback Method
log10ws	-2.23		Crippen Method
logp	1.890		Crippen Method
mcvol	171.060	ml/mol	McGowan Method
pc	2487.55	kPa	Joback Method
rinpol	1873.00		NIST Webbook
rinpol	1834.00		NIST Webbook
rinpol	1873.00		NIST Webbook
rinpol	1873.00		NIST Webbook
rinpol	1825.00		NIST Webbook
rinpol	1895.30		NIST Webbook
rinpol	1834.00		NIST Webbook
tb	635.89	K	Joback Method
tc	847.87	K	Joback Method
tf	388.00	K	Joback Method
vc	0.639	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	422.99	J/mol×K	635.89	Joback Method
cpg	436.66	J/mol×K	671.22	Joback Method
cpg	449.59	J/mol×K	706.55	Joback Method
cpg	461.77	J/mol×K	741.88	Joback Method
cpg	473.21	J/mol×K	777.21	Joback Method
cpg	483.89	J/mol×K	812.54	Joback Method
cpg	493.81	J/mol×K	847.87	Joback Method
dvisc	0.0006990	Pa×s	388.00	Joback Method
dvisc	0.0004299	Pa×s	429.31	Joback Method
dvisc	0.0002880	Pa×s	470.63	Joback Method
dvisc	0.0002058	Pa×s	511.94	Joback Method
dvisc	0.0001546	Pa×s	553.26	Joback Method
dvisc	0.0001209	Pa×s	594.58	Joback Method
dvisc	0.0000976	Pa×s	635.89	Joback Method

Sources

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
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C5396645&Units=SI

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