2-Propenoic acid, 3-(3,4,5-trimethoxyphenyl)-, methyl ester, cis

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-ALCCZGGFSA-N

Formula: C12H14O4

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

Mol. weight [g/mol]: 222.24

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	1851.00		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

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R298436&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