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

Other names: Cinnamic acid, 3,4,5-trimethoxy-, methyl ester
Methyl 3,4,5-trimethoxycinnamate
Methyl ester of 3,4,5-Trimethoxycinnamic acid
Sinapic acid, O,O'-dimethyl-
Methyl (2E)-3-(3,4,5-trimethoxyphenyl)-2-propenoate
2-Propenoic acid, 3-(3,4,5-trimethoxyphenyl)-, methyl ester, trans

Inchi: InChI=1S/C13H16O5/c1-15-10-7-9(5-6-12(14)17-3)8-11(16-2)13(10)18-4/h5-8H,1-4H3/b

InchiKey: KLXHCGFNNUQTEY-AATRIKPKSA-N

Formula: C13H16O5

SMILES: COC(=O)C=Cc1cc(OC)c(OC)c(OC)c1

Mol. weight [g/mol]: 252.26

CAS: 7560-49-8

Physical Properties

Property code	Value	Unit	Source
gf	-326.60	kJ/mol	Joback Method
hf	-633.77	kJ/mol	Joback Method
hfus	28.85	kJ/mol	Joback Method
hvap	65.14	kJ/mol	Joback Method
log10ws	-2.35		Crippen Method
logp	1.899		Crippen Method
mcvol	191.020	ml/mol	McGowan Method
pc	2197.95	kPa	Joback Method
rinpol	2030.00		NIST Webbook
rinpol	1966.00		NIST Webbook
tb	686.17	K	Joback Method
tc	893.75	K	Joback Method
tf	434.02	K	Joback Method
vc	0.714	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	498.43	J/mol×K	686.17	Joback Method

cpg	560.19	J/mol×K	859.15	Joback Method
cpg	549.47	J/mol×K	824.56	Joback Method
cpg	537.90	J/mol×K	789.96	Joback Method
cpg	525.53	J/mol×K	755.36	Joback Method
cpg	512.36	J/mol×K	720.77	Joback Method
cpg	570.06	J/mol×K	893.75	Joback Method
dvisc	0.0000688	Pa×s	686.17	Joback Method
dvisc	0.0000842	Pa×s	644.15	Joback Method
dvisc	0.0001060	Pa×s	602.12	Joback Method
dvisc	0.0001381	Pa×s	560.10	Joback Method
dvisc	0.0001879	Pa×s	518.07	Joback Method
dvisc	0.0002698	Pa×s	476.05	Joback Method
dvisc	0.0004157	Pa×s	434.02	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=C7560498&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
rinpol: Non-polar retention indices
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point

vc: Critical Volume