2-Propenoic, 3-(3, 4, 5 trimethoxy phenyl) methylester

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

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	1784.00		NIST Webbook
rinpol	1784.00		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	512.36	J/mol×K	720.77	Joback Method
cpg	525.53	J/mol×K	755.36	Joback Method
cpg	537.90	J/mol×K	789.96	Joback Method
cpg	549.47	J/mol×K	824.56	Joback Method
cpg	560.19	J/mol×K	859.15	Joback Method
cpg	570.06	J/mol×K	893.75	Joback Method
dvisc	0.0004157	Pa×s	434.02	Joback Method

dvisc	0.0002698	Pa×s	476.05	Joback Method
dvisc	0.0001879	Pa×s	518.07	Joback Method
dvisc	0.0001381	Pa×s	560.10	Joback Method
dvisc	0.0001060	Pa×s	602.12	Joback Method
dvisc	0.0000842	Pa×s	644.15	Joback Method
dvisc	0.0000688	Pa×s	686.17	Joback Method

Sources

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=R417548&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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