Propanoic acid, 3-(3,4,5-trimethoxyphenyl), methyl ester

Inchi: InChI=1S/C13H18O5/c1-15-10-7-9(5-6-12(14)17-3)8-11(16-2)13(10)18-4/h7-8H,5-6H2,1-

InchiKey: KCQHYTFTCZDNMC-UHFFFAOYSA-N

Formula: C13H18O5

SMILES: COC(=O)CCc1cc(OC)c(OC)c(OC)c1

Mol. weight [g/mol]: 254.28

Physical Properties

Property code	Value	Unit	Source
gf	-406.82	kJ/mol	Joback Method
hf	-750.99	kJ/mol	Joback Method
hfus	28.65	kJ/mol	Joback Method
hvap	65.18	kJ/mol	Joback Method
log10ws	-2.33		Crippen Method
logp	1.818		Crippen Method
mcvol	195.320	ml/mol	McGowan Method
pc	2094.58	kPa	Joback Method
rinpol	1815.00		NIST Webbook
tb	682.01	K	Joback Method
tc	882.39	K	Joback Method
tf	439.10	K	Joback Method
vc	0.734	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	521.18	J/mol×K	682.01	Joback Method
cpg	535.66	J/mol×K	715.41	Joback Method
cpg	549.38	J/mol×K	748.80	Joback Method
cpg	562.32	J/mol×K	782.20	Joback Method
cpg	574.45	J/mol×K	815.59	Joback Method
cpg	585.73	J/mol×K	848.99	Joback Method
cpg	596.13	J/mol×K	882.39	Joback Method
dvisc	0.0004555	Pa×s	439.10	Joback Method
dvisc	0.0003014	Pa×s	479.59	Joback Method

dvisc	0.0002126	Pa×s	520.07	Joback Method
dvisc	0.0001578	Pa×s	560.56	Joback Method
dvisc	0.0001219	Pa×s	601.04	Joback Method
dvisc	0.0000973	Pa×s	641.52	Joback Method
dvisc	0.0000797	Pa×s	682.01	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=R220923&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