Ethyl 3-(3,4-dimethoxyphenyl)acrylate

Inchi: InChI=1S/C13H16O4/c1-4-17-13(14)8-6-10-5-7-11(15-2)12(9-10)16-3/h5-9H,4H2,1-3H3/
InchiKey: SUFLQJBENWTBOL-SOFGYWHQSA-N
Formula: C13H16O4
SMILES: CCOC(=O)C=Cc1ccc(OC)c(OC)c1
Mol. weight [g/mol]: 236.26
CAS: 20583-78-2

Physical Properties

Property code	Value	Unit	Source
gf	-211.97	kJ/mol	Joback Method
hf	-490.08	kJ/mol	Joback Method
hfus	28.05	kJ/mol	Joback Method
hvap	62.07	kJ/mol	Joback Method
log10ws	-2.65		Crippen Method
logp	2.280		Crippen Method
mcvol	185.150	ml/mol	McGowan Method
pc	2265.42	kPa	Joback Method
rinpol	1968.30		NIST Webbook
rinpol	1968.30		NIST Webbook
tb	658.77	K	Joback Method
tc	867.49	K	Joback Method
tf	399.27	K	Joback Method
vc	0.696	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	473.40	J/mol×K	658.77	Joback Method
cpg	487.70	J/mol×K	693.56	Joback Method
cpg	501.21	J/mol×K	728.34	Joback Method
cpg	513.93	J/mol×K	763.13	Joback Method
cpg	525.86	J/mol×K	797.92	Joback Method
cpg	536.99	J/mol×K	832.70	Joback Method
cpg	547.32	J/mol×K	867.49	Joback Method

dvisc	0.0006686	Pa×s	399.27	Joback Method
dvisc	0.0004044	Pa×s	442.52	Joback Method
dvisc	0.0002675	Pa×s	485.77	Joback Method
dvisc	0.0001893	Pa×s	529.02	Joback Method
dvisc	0.0001412	Pa×s	572.27	Joback Method
dvisc	0.0001097	Pa×s	615.52	Joback Method
dvisc	0.0000881	Pa×s	658.77	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=C20583782&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