di-(3-Methoxybutyl)oxalate

Inchi: InChI=1S/C12H22O6/c1-9(15-3)5-7-17-11(13)12(14)18-8-6-10(2)16-4/h9-10H,5-8H2,1-4
InchiKey: ANHIFMIRJGTUHE-UHFFFAOYSA-N
Formula: C12H22O6
SMILES: COC(C)CCOC(=O)C(=O)OCCC(C)OC
Mol. weight [g/mol]: 262.30

Physical Properties

Property code	Value	Unit	Source
gf	-632.56	kJ/mol	Joback Method
hf	-1055.61	kJ/mol	Joback Method
hfus	27.74	kJ/mol	Joback Method
hvap	64.66	kJ/mol	Joback Method
log10ws	-0.97		Crippen Method
logp	0.923		Crippen Method
mcvol	206.560	ml/mol	McGowan Method
pc	1896.95	kPa	Joback Method
rinpol	1619.00		NIST Webbook
rinpol	1619.00		NIST Webbook
tb	670.50	K	Joback Method
tc	852.67	K	Joback Method
tf	383.78	K	Joback Method
vc	0.779	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	571.78	J/mol×K	670.50	Joback Method
cpg	586.51	J/mol×K	700.86	Joback Method
cpg	600.54	J/mol×K	731.22	Joback Method
cpg	613.86	J/mol×K	761.58	Joback Method
cpg	626.44	J/mol×K	791.94	Joback Method
cpg	638.28	J/mol×K	822.31	Joback Method
cpg	649.34	J/mol×K	852.67	Joback Method
dvisc	0.0012699	Pa×s	383.78	Joback Method

dvisc	0.0006179	Pa×s	431.57	Joback Method
dvisc	0.0003471	Pa×s	479.35	Joback Method
dvisc	0.0002165	Pa×s	527.14	Joback Method
dvisc	0.0001460	Pa×s	574.93	Joback Method
dvisc	0.0001046	Pa×s	622.71	Joback Method
dvisc	0.0000786	Pa×s	670.50	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R542248&Units=SI

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