di-(3-Methoxybutyl)malonate

Inchi: InChI=1S/C13H24O6/c1-10(16-3)5-7-18-12(14)9-13(15)19-8-6-11(2)17-4/h10-11H,5-9H2
InchiKey: GUDJNYIITYNNFQ-UHFFFAOYSA-N
Formula: C13H24O6
SMILES: COC(C)CCOC(=O)CC(=O)OCCC(C)OC
Mol. weight [g/mol]: 276.33

Physical Properties

Property code	Value	Unit	Source
gf	-624.14	kJ/mol	Joback Method
hf	-1076.25	kJ/mol	Joback Method
hfus	30.33	kJ/mol	Joback Method
hvap	66.89	kJ/mol	Joback Method
log10ws	-1.39		Crippen Method
logp	1.313		Crippen Method
mcvol	220.650	ml/mol	McGowan Method
pc	1747.74	kPa	Joback Method
rinpol	1699.00		NIST Webbook
rinpol	1699.00		NIST Webbook
tb	693.38	K	Joback Method
tc	874.82	K	Joback Method
tf	395.05	K	Joback Method
vc	0.836	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	625.72	J/mol×K	693.38	Joback Method
cpg	694.16	J/mol×K	844.58	Joback Method
cpg	682.05	J/mol×K	814.34	Joback Method
cpg	669.14	J/mol×K	784.10	Joback Method
cpg	655.43	J/mol×K	753.86	Joback Method
cpg	640.95	J/mol×K	723.62	Joback Method
cpg	705.45	J/mol×K	874.82	Joback Method
dvisc	0.0000688	Pa×s	693.38	Joback Method

dvisc	0.0000918	Pa×s	643.66	Joback Method
dvisc	0.0001286	Pa×s	593.94	Joback Method
dvisc	0.0001915	Pa×s	544.22	Joback Method
dvisc	0.0003091	Pa×s	494.49	Joback Method
dvisc	0.0005552	Pa×s	444.77	Joback Method
dvisc	0.0011558	Pa×s	395.05	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=R542233&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

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