di-(1-Methyl-2-methoxybutyl)malonate

Inchi: InChI=1S/C13H24O6/c1-8(16-5)10(3)18-12(14)7-13(15)19-11(4)9(2)17-6/h8-11H,7H2,1-
InchiKey: CFGKAIVHVIEZKM-UHFFFAOYSA-N
Formula: C13H24O6
SMILES: COC(C)C(C)OC(=O)CC(=O)OC(C)C(C)OC
Mol. weight [g/mol]: 276.33

Physical Properties

Property code	Value	Unit	Source
gf	-629.02	kJ/mol	Joback Method
hf	-1086.81	kJ/mol	Joback Method
hfus	23.28	kJ/mol	Joback Method
hvap	66.11	kJ/mol	Joback Method
log10ws	-1.61		Crippen Method
logp	1.310		Crippen Method
mcvol	220.650	ml/mol	McGowan Method
pc	1771.36	kPa	Joback Method
rinpol	1477.00		NIST Webbook
tb	692.50	K	Joback Method
tc	878.99	K	Joback Method
tf	365.05	K	Joback Method
vc	0.824	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	626.70	J/mol×K	692.50	Joback Method
cpg	642.41	J/mol×K	723.58	Joback Method
cpg	657.30	J/mol×K	754.66	Joback Method
cpg	671.36	J/mol×K	785.74	Joback Method
cpg	684.57	J/mol×K	816.83	Joback Method
cpg	696.91	J/mol×K	847.91	Joback Method
cpg	708.36	J/mol×K	878.99	Joback Method
dvisc	0.0018644	Pa×s	365.05	Joback Method
dvisc	0.0007210	Pa×s	419.62	Joback Method

dvisc	0.0003470	Pa×s	474.20	Joback Method
dvisc	0.0001942	Pa×s	528.77	Joback Method
dvisc	0.0001212	Pa×s	583.35	Joback Method
dvisc	0.0000820	Pa×s	637.92	Joback Method
dvisc	0.0000590	Pa×s	692.50	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=R541849&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