

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
mvol	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	m ³ /kmol	Joback Method

Temperature Dependent Properties

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

dvisc	0.0000918	Paxs	643.66	Joback Method
dvisc	0.0001286	Paxs	593.94	Joback Method
dvisc	0.0001915	Paxs	544.22	Joback Method
dvisc	0.0003091	Paxs	494.49	Joback Method
dvisc	0.0005552	Paxs	444.77	Joback Method
dvisc	0.0011558	Paxs	395.05	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R542233&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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

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
mccvol:	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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