

Dimethylmalonic acid, ethyl isoheptyl ester

Inchi:	InChI=1S/C13H24O4/c1-6-16-11(14)13(4,5)12(15)17-9-7-8-10(2)3/h10H,6-9H2,1-5H3
InchiKey:	QDQYWWRVYXQNWQH-UHFFFAOYSA-N
Formula:	C13H24O4
SMILES:	CCOC(=O)C(C)(C)C(=O)OCCCC(C)C
Mol. weight [g/mol]:	244.33

Physical Properties

Property code	Value	Unit	Source
gf	-408.86	kJ/mol	Joback Method
hf	-815.28	kJ/mol	Joback Method
hfus	24.06	kJ/mol	Joback Method
hvap	61.16	kJ/mol	Joback Method
log10ws	-2.51		Crippen Method
logp	2.555		Crippen Method
mcvol	208.910	ml/mol	McGowan Method
pc	1815.41	kPa	Joback Method
rinpol	1434.00		NIST Webbook
tb	645.75	K	Joback Method
tc	832.89	K	Joback Method
tf	368.01	K	Joback Method
vc	0.794	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	571.62	J/molxK	645.75	Joback Method
cpg	643.16	J/molxK	801.70	Joback Method
cpg	630.43	J/molxK	770.51	Joback Method
cpg	616.93	J/molxK	739.32	Joback Method
cpg	602.64	J/molxK	708.13	Joback Method
cpg	587.54	J/molxK	676.94	Joback Method
cpg	655.14	J/molxK	832.89	Joback Method
dvisc	0.0001090	Paxs	645.75	Joback Method
dvisc	0.0001478	Paxs	599.46	Joback Method

dvisc	0.0002110	Paxs	553.17	Joback Method
dvisc	0.0003214	Paxs	506.88	Joback Method
dvisc	0.0005328	Paxs	460.59	Joback Method
dvisc	0.0009889	Paxs	414.30	Joback Method
dvisc	0.0021445	Paxs	368.01	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U361715&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

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