

Dimethylmalonic acid, heptyl isobutyl ester

Inchi:	InChI=1S/C16H30O4/c1-6-7-8-9-10-11-19-14(17)16(4,5)15(18)20-12-13(2)3/h13H,6-12H
InchiKey:	KRMQTRAAENYFIR-UHFFFAOYSA-N
Formula:	C16H30O4
SMILES:	CCCCCCCOC(=O)C(C)(C)C(=O)OCC(C)C
Mol. weight [g/mol]:	286.41

Physical Properties

Property code	Value	Unit	Source
gf	-383.60	kJ/mol	Joback Method
hf	-877.20	kJ/mol	Joback Method
hfus	31.83	kJ/mol	Joback Method
hvap	67.84	kJ/mol	Joback Method
log10ws	-3.76		Crippen Method
logp	3.725		Crippen Method
mcvol	251.180	ml/mol	McGowan Method
pc	1440.25	kPa	Joback Method
rinpol	1700.00		NIST Webbook
tb	714.39	K	Joback Method
tc	898.38	K	Joback Method
tf	401.82	K	Joback Method
vc	0.963	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	736.17	J/molxK	714.39	Joback Method
cpg	753.26	J/molxK	745.06	Joback Method
cpg	769.43	J/molxK	775.72	Joback Method
cpg	784.70	J/molxK	806.39	Joback Method
cpg	799.10	J/molxK	837.05	Joback Method
cpg	812.65	J/molxK	867.72	Joback Method
cpg	825.37	J/molxK	898.38	Joback Method
dvisc	0.0015604	Paxs	401.82	Joback Method
dvisc	0.0006949	Paxs	453.91	Joback Method

dvisc	0.0003656	Paxs	506.01	Joback Method
dvisc	0.0002168	Paxs	558.11	Joback Method
dvisc	0.0001406	Paxs	610.20	Joback Method
dvisc	0.0000976	Paxs	662.30	Joback Method
dvisc	0.0000715	Paxs	714.39	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U361655&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
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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