Dimethylmalonic acid, hexyl 3-methylbutyl ester

Inchi: InChI=1S/C16H30O4/c1-6-7-8-9-11-19-14(17)16(4,5)15(18)20-12-10-13(2)3/h13H,6-12H

InchiKey: JGHADYSDZWSCSS-UHFFFAOYSA-N

Formula: C16H30O4

SMILES: CCCCCCOC(=O)C(C)(C)C(=O)OCCC(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	1694.00		NIST Webbook
rinpol	1694.00		NIST Webbook
tb	714.39	K	Joback Method
tc	898.38	K	Joback Method
tf	401.82	K	Joback Method
vc	0.963	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	736.17	J/mol×K	714.39	Joback Method
cpg	753.26	J/mol×K	745.06	Joback Method
cpg	769.43	J/mol×K	775.72	Joback Method
cpg	784.70	J/mol×K	806.39	Joback Method
cpg	799.10	J/mol×K	837.05	Joback Method
cpg	812.65	J/mol×K	867.72	Joback Method
cpg	825.37	J/mol×K	898.38	Joback Method
dvisc	0.0015604	Pa×s	401.82	Joback Method

dvisc	0.0006949	Pa×s	453.91	Joback Method
dvisc	0.0003656	Pa×s	506.01	Joback Method
dvisc	0.0002168	Pa×s	558.11	Joback Method
dvisc	0.0001406	Pa×s	610.20	Joback Method
dvisc	0.0000976	Pa×s	662.30	Joback Method
dvisc	0.0000715	Pa×s	714.39	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=U361595&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