Dimethylmalonic acid, isohexyl neopentyl ester

Inchi: InChI=1S/C16H30O4/c1-12(2)9-8-10-19-13(17)16(6,7)14(18)20-11-15(3,4)5/h12H,8-11H

InchiKey: JJFJHQHPSDVDJF-UHFFFAOYSA-N

Formula: C16H30O4

SMILES: CC(C)CCCOC(=O)C(C)(C)C(=O)OCC(C)(C)C

Mol. weight [g/mol]: 286.41

Physical Properties

Property code	Value	Unit	Source
gf	-380.76	kJ/mol	Joback Method
hf	-885.95	kJ/mol	Joback Method
hfus	24.42	kJ/mol	Joback Method
hvap	66.54	kJ/mol	Joback Method
log10ws	-3.52		Crippen Method
logp	3.581		Crippen Method
mcvol	251.180	ml/mol	McGowan Method
pc	1461.25	kPa	Joback Method
rinpol	1605.00		NIST Webbook
tb	711.16	K	Joback Method
tc	902.13	K	Joback Method
tf	404.24	K	Joback Method
vc	0.952	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	738.31	J/mol×K	711.16	Joback Method
cpg	755.81	J/mol×K	742.99	Joback Method
cpg	772.30	J/mol×K	774.82	Joback Method
cpg	787.81	J/mol×K	806.64	Joback Method
cpg	802.39	J/mol×K	838.47	Joback Method
cpg	816.07	J/mol×K	870.30	Joback Method
cpg	828.88	J/mol×K	902.13	Joback Method
dvisc	0.0015901	Pa×s	404.24	Joback Method
dvisc	0.0006771	Pa×s	455.39	Joback Method

dvisc	0.0003426	Pa×s	506.55	Joback Method
dvisc	0.0001964	Pa×s	557.70	Joback Method
dvisc	0.0001236	Pa×s	608.85	Joback Method
dvisc	0.0000836	Pa×s	660.01	Joback Method
dvisc	0.0000598	Pa×s	711.16	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U361746&Units=SI

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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