Dimethylmalonic acid, isohexyl 2-pentyl ester

Inchi: InChI=1S/C16H30O4/c1-7-9-13(4)20-15(18)16(5,6)14(17)19-11-8-10-12(2)3/h12-13H,7-1
InchiKey: NHLNWTNZZXFAIY-UHFFFAOYSA-N
Formula: C16H30O4
SMILES: CCCC(C)OC(=O)C(C)(C)C(=O)OCCCC(C)C
Mol. weight [g/mol]: 286.41

Physical Properties

Property code	Value	Unit	Source
gf	-386.04	kJ/mol	Joback Method
hf	-882.48	kJ/mol	Joback Method
hfus	28.31	kJ/mol	Joback Method
hvap	67.45	kJ/mol	Joback Method
log10ws	-3.87		Crippen Method
logp	3.724		Crippen Method
mcvol	251.180	ml/mol	McGowan Method
pc	1449.04	kPa	Joback Method
rinpol	1661.00		NIST Webbook
tb	713.95	K	Joback Method
tc	900.32	K	Joback Method
tf	386.82	K	Joback Method
vc	0.957	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	736.65	J/mol×K	713.95	Joback Method
cpg	753.98	J/mol×K	745.01	Joback Method
cpg	770.36	J/mol×K	776.07	Joback Method
cpg	785.81	J/mol×K	807.13	Joback Method
cpg	800.36	J/mol×K	838.20	Joback Method
cpg	814.03	J/mol×K	869.26	Joback Method
cpg	826.83	J/mol×K	900.32	Joback Method
dvisc	0.0019778	Pa×s	386.82	Joback Method
dvisc	0.0007910	Pa×s	441.34	Joback Method

dvisc	0.0003870	Pa×s	495.86	Joback Method
dvisc	0.0002181	Pa×s	550.38	Joback Method
dvisc	0.0001363	Pa×s	604.91	Joback Method
dvisc	0.0000921	Pa×s	659.43	Joback Method
dvisc	0.0000661	Pa×s	713.95	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U361582&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

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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