

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-
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
rinsol	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	m ³ /kmol	Joback Method

Temperature Dependent Properties

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

dvisc	0.0003870	Paxs	495.86	Joback Method
dvisc	0.0002181	Paxs	550.38	Joback Method
dvisc	0.0001363	Paxs	604.91	Joback Method
dvisc	0.0000921	Paxs	659.43	Joback Method
dvisc	0.0000661	Paxs	713.95	Joback Method

Sources

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=U361582&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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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