

# Dimethylmalonic acid, isohexyl pentyl ester

<b>Inchi:</b>	InChI=1S/C16H30O4/c1-6-7-8-11-19-14(17)16(4,5)15(18)20-12-9-10-13(2)3/h13H,6-12H
<b>InchiKey:</b>	KQHCIDIUMGZKJOS-UHFFFAOYSA-N
<b>Formula:</b>	C16H30O4
<b>SMILES:</b>	CCCCCOC(=O)C(C)(C)C(=O)OCCCC(C)C
<b>Mol. weight [g/mol]:</b>	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	1696.00		NIST Webbook
tb	714.39	K	Joback Method
tc	898.38	K	Joback Method
tf	401.82	K	Joback Method
vc	0.963	m <sup>3</sup> /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

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=U361717&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U361717&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</a>
<b>Crippen Method:</b>	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>
<b>Joback Method:</b>	<a href="https://en.wikipedia.org/wiki/Joback_method">https://en.wikipedia.org/wiki/Joback_method</a>
<b>McGowan Method:</b>	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>

## Legend

<b>cpg:</b>	Ideal gas heat capacity
<b>dvisc:</b>	Dynamic viscosity
<b>gf:</b>	Standard Gibbs free energy of formation
<b>hf:</b>	Enthalpy of formation at standard conditions
<b>hfus:</b>	Enthalpy of fusion at standard conditions
<b>hvap:</b>	Enthalpy of vaporization at standard conditions
<b>log10ws:</b>	Log10 of Water solubility in mol/l
<b>logp:</b>	Octanol/Water partition coefficient
<b>mcvol:</b>	McGowan's characteristic volume
<b>pc:</b>	Critical Pressure
<b>rinpol:</b>	Non-polar retention indices
<b>tb:</b>	Normal Boiling Point Temperature
<b>tc:</b>	Critical Temperature
<b>tf:</b>	Normal melting (fusion) point
<b>vc:</b>	Critical Volume

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