

# Dimethylmalonic acid, hexyl neopentyl ester

<b>Inchi:</b>	InChI=1S/C16H30O4/c1-7-8-9-10-11-19-13(17)16(5,6)14(18)20-12-15(2,3)4/h7-12H2,1-6
<b>InchiKey:</b>	SXWZOARAXWPTRG-UHFFFAOYSA-N
<b>Formula:</b>	C16H30O4
<b>SMILES:</b>	CCCCCOC(=O)C(C)(C)C(=O)OCC(C)(C)C
<b>Mol. weight [g/mol]:</b>	286.41

## Physical Properties

Property code	Value	Unit	Source
gf	-378.32	kJ/mol	Joback Method
hf	-880.67	kJ/mol	Joback Method
hfus	27.94	kJ/mol	Joback Method
hvap	66.93	kJ/mol	Joback Method
log10ws	-3.76		Crippen Method
logp	3.725		Crippen Method
mcvol	251.180	ml/mol	McGowan Method
pc	1452.35	kPa	Joback Method
rinpol	1642.00		NIST Webbook
rinpol	1642.00		NIST Webbook
tb	711.60	K	Joback Method
tc	899.93	K	Joback Method
tf	419.24	K	Joback Method
vc	0.958	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	737.83	J/molxK	711.60	Joback Method
cpg	755.07	J/molxK	742.99	Joback Method
cpg	771.33	J/molxK	774.38	Joback Method
cpg	786.65	J/molxK	805.77	Joback Method
cpg	801.07	J/molxK	837.16	Joback Method
cpg	814.62	J/molxK	868.55	Joback Method
cpg	827.34	J/molxK	899.93	Joback Method
dvisc	0.0012657	Paxs	419.24	Joback Method

dvisc	0.0005957	Paxs	467.97	Joback Method
dvisc	0.0003232	Paxs	516.69	Joback Method
dvisc	0.0001948	Paxs	565.42	Joback Method
dvisc	0.0001273	Paxs	614.15	Joback Method
dvisc	0.0000885	Paxs	662.87	Joback Method
dvisc	0.0000647	Paxs	711.60	Joback Method

## Sources

<b>McGowan Method:</b>	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=U361747&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U361747&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>

## Legend

<b>cp<sub>g</sub>:</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>log<sub>10</sub>ws:</b>	Log <sub>10</sub> of Water solubility in mol/l
<b>logp:</b>	Octanol/Water partition coefficient
<b>m<sub>cvol</sub>:</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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