

# Dimethylmalonic acid, hexadecyl hexyl ester

**Inchi:** InChI=1S/C27H52O4/c1-5-7-9-11-12-13-14-15-16-17-18-19-20-22-24-31-26(29)27(3,4)2  
**InchiKey:** MOLVUMVMQISKJJ-UHFFFAOYSA-N  
**Formula:** C27H52O4  
**SMILES:** CCCCCCCCCCCCCCOC(=O)C(C)(C)C(=O)OCCCCC  
**Mol. weight [g/mol]:** 440.70

## Physical Properties

Property code	Value	Unit	Source
gf	-288.54	kJ/mol	Joback Method
hf	-1098.96	kJ/mol	Joback Method
hfus	63.85	kJ/mol	Joback Method
hvap	92.71	kJ/mol	Joback Method
log10ws	-8.61		Crippen Method
logp	8.161		Crippen Method
mvol	406.170	ml/mol	McGowan Method
pc	730.86	kPa	Joback Method
rinpol	2802.00		NIST Webbook
rinpol	2802.00		NIST Webbook
tb	966.51	K	Joback Method
tc	1190.06	K	Joback Method
tf	540.79	K	Joback Method
vc	1.585	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1409.34	J/molxK	966.51	Joback Method
cpg	1501.45	J/molxK	1152.80	Joback Method
cpg	1486.00	J/molxK	1115.54	Joback Method
cpg	1469.14	J/molxK	1078.28	Joback Method
cpg	1450.80	J/molxK	1041.03	Joback Method
cpg	1430.89	J/molxK	1003.77	Joback Method
cpg	1515.58	J/molxK	1190.06	Joback Method
dvisc	0.0000141	Paxs	966.51	Joback Method

dvisc	0.0000192	Paxs	895.56	Joback Method
dvisc	0.0000278	Paxs	824.60	Joback Method
dvisc	0.0000431	Paxs	753.65	Joback Method
dvisc	0.0000730	Paxs	682.70	Joback Method
dvisc	0.0001400	Paxs	611.74	Joback Method
dvisc	0.0003183	Paxs	540.79	Joback Method

## Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=U361697&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U361697&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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