

# Diethylmalonic acid, hexyl propyl ester

<b>Inchi:</b>	InChI=1S/C16H30O4/c1-5-9-10-11-13-20-15(18)16(7-3,8-4)14(17)19-12-6-2/h5-13H2,1-4
<b>InchiKey:</b>	ZACZNHWHDXQAY-UHFFFAOYSA-N
<b>Formula:</b>	C16H30O4
<b>SMILES:</b>	CCCCCOC(=O)C(CC)(CC)C(=O)OCCC
<b>Mol. weight [g/mol]:</b>	286.41

## Physical Properties

Property code	Value	Unit	Source
gf	-381.16	kJ/mol	Joback Method
hf	-871.92	kJ/mol	Joback Method
hfus	35.36	kJ/mol	Joback Method
hvap	68.23	kJ/mol	Joback Method
log10ws	-4.00		Crippen Method
logp	3.870		Crippen Method
mcvol	251.180	ml/mol	McGowan Method
pc	1431.55	kPa	Joback Method
rinpol	1691.00		NIST Webbook
rinpol	1691.00		NIST Webbook
tb	714.83	K	Joback Method
tc	896.57	K	Joback Method
tf	416.82	K	Joback Method
vc	0.969	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	735.69	J/molxK	714.83	Joback Method
cpg	811.32	J/molxK	866.28	Joback Method
cpg	797.88	J/molxK	835.99	Joback Method
cpg	783.62	J/molxK	805.70	Joback Method
cpg	768.52	J/molxK	775.41	Joback Method
cpg	752.55	J/molxK	745.12	Joback Method
cpg	823.95	J/molxK	896.57	Joback Method
dvisc	0.0000773	Paxs	714.83	Joback Method

dvisc	0.0001035	Paxs	665.16	Joback Method
dvisc	0.0001453	Paxs	615.49	Joback Method
dvisc	0.0002164	Paxs	565.82	Joback Method
dvisc	0.0003480	Paxs	516.16	Joback Method
dvisc	0.0006193	Paxs	466.49	Joback Method
dvisc	0.0012644	Paxs	416.82	Joback Method

## Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=U369438&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U369438&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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