

# Diethylmalonic acid, hexadecyl 3-methylpentyl ester

Inchi:	InChI=1S/C29H56O4/c1-6-10-11-12-13-14-15-16-17-18-19-20-21-22-24-32-27(30)29(8-3
InchiKey:	OJYRCVVYGNIP EU-UHFFFAOYSA-N
Formula:	C29H56O4
SMILES:	CCCCCCCCCCCCCCCCOC(=O)C(CC)(CC)C(=O)OCCC(C)CC
Mol. weight [g/mol]:	468.75

## Physical Properties

Property code	Value	Unit	Source
gf	-274.14	kJ/mol	Joback Method
hf	-1145.52	kJ/mol	Joback Method
hfus	65.50	kJ/mol	Joback Method
hvap	96.78	kJ/mol	Joback Method
log10ws	-9.20		Crippen Method
logp	8.797		Crippen Method
mcvol	434.350	ml/mol	McGowan Method
pc	663.23	kPa	Joback Method
rinpol	2845.00		NIST Webbook
tb	1011.83	K	Joback Method
tc	1253.72	K	Joback Method
tf	548.33	K	Joback Method
vc	1.690	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1539.55	J/molxK	1011.83	Joback Method
cpg	1634.74	J/molxK	1213.40	Joback Method
cpg	1619.12	J/molxK	1173.09	Joback Method
cpg	1601.90	J/molxK	1132.77	Joback Method
cpg	1582.97	J/molxK	1092.46	Joback Method
cpg	1562.22	J/molxK	1052.14	Joback Method
cpg	1648.87	J/molxK	1253.72	Joback Method
dvisc	0.0000092	Paxs	1011.83	Joback Method
dvisc	0.0000128	Paxs	934.58	Joback Method

dvisc	0.0000189	Paxs	857.33	Joback Method
dvisc	0.0000303	Paxs	780.08	Joback Method
dvisc	0.0000536	Paxs	702.83	Joback Method
dvisc	0.0001093	Paxs	625.58	Joback Method
dvisc	0.0002725	Paxs	548.33	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=U370602&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U370602&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>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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