

# Diethylmalonic acid, 3-methylbutyl octadecyl ester

Inchi:	InChI=1S/C30H58O4/c1-6-9-10-11-12-13-14-15-16-17-18-19-20-21-22-23-25-33-28(31)3
InchiKey:	ZDIYPLQESPWGRY-UHFFFAOYSA-N
Formula:	C30H58O4
SMILES:	CCCCCCCCCCCCCCCCCOC(=O)C(CC)(CC)C(=O)OCCC(C)C
Mol. weight [g/mol]:	482.78

## Physical Properties

Property code	Value	Unit	Source
gf	-265.72	kJ/mol	Joback Method
hf	-1166.16	kJ/mol	Joback Method
hfus	68.09	kJ/mol	Joback Method
hvap	99.00	kJ/mol	Joback Method
log10ws	-9.62		Crippen Method
logp	9.187		Crippen Method
mcvol	448.440	ml/mol	McGowan Method
pc	631.61	kPa	Joback Method
rinpol	3040.00		NIST Webbook
rinpol	3040.00		NIST Webbook
tb	1034.71	K	Joback Method
tc	1288.59	K	Joback Method
tf	559.60	K	Joback Method
vc	1.746	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1604.99	J/molxK	1034.71	Joback Method
cpg	1702.40	J/molxK	1246.28	Joback Method
cpg	1686.61	J/molxK	1203.97	Joback Method
cpg	1669.10	J/molxK	1161.65	Joback Method
cpg	1649.75	J/molxK	1119.34	Joback Method
cpg	1628.42	J/molxK	1077.02	Joback Method
cpg	1716.62	J/molxK	1288.59	Joback Method
dvisc	0.0000078	Paxs	1034.71	Joback Method

dvisc	0.0000109	Paxs	955.52	Joback Method
dvisc	0.0000161	Paxs	876.34	Joback Method
dvisc	0.0000257	Paxs	797.15	Joback Method
dvisc	0.0000457	Paxs	717.97	Joback Method
dvisc	0.0000935	Paxs	638.78	Joback Method
dvisc	0.0002345	Paxs	559.60	Joback Method

## Sources

<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>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=U369397&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U369397&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307l">http://pubs.acs.org/doi/abs/10.1021/ci990307l</a>

## Legend

<b>cp<sub>g</sub>:</b>	Ideal gas heat capacity
<b>dvisc:</b>	Dynamic viscosity
<b>g<sub>f</sub>:</b>	Standard Gibbs free energy of formation
<b>h<sub>f</sub>:</b>	Enthalpy of formation at standard conditions
<b>h<sub>fus</sub>:</b>	Enthalpy of fusion at standard conditions
<b>h<sub>vap</sub>:</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>log<sub>p</sub>:</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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