

# Diethylmalonic acid, heptyl octadecyl ester

<b>Inchi:</b>	InChI=1S/C32H62O4/c1-5-9-11-13-14-15-16-17-18-19-20-21-22-23-25-27-29-36-31(34)3
<b>InchiKey:</b>	ZWCGPJKRXSOLSF-UHFFFAOYSA-N
<b>Formula:</b>	C32H62O4
<b>SMILES:</b>	CCCCCCCCCCCCCCCCCOC(=O)C(CC)(CC)C(=O)OCCCCCCC
<b>Mol. weight [g/mol]:</b>	510.83

## Physical Properties

Property code	Value	Unit	Source
gf	-246.44	kJ/mol	Joback Method
hf	-1202.16	kJ/mol	Joback Method
hfus	76.80	kJ/mol	Joback Method
hvap	103.84	kJ/mol	Joback Method
log10ws	-10.70		Crippen Method
logp	10.111		Crippen Method
mcvol	476.620	ml/mol	McGowan Method
pc	572.61	kPa	Joback Method
rinqol	3263.00		NIST Webbook
tb	1080.91	K	Joback Method
tc	1367.66	K	Joback Method
tf	597.14	K	Joback Method
vc	1.865	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1736.61	J/molxK	1080.91	Joback Method
cpg	1762.24	J/molxK	1128.70	Joback Method
cpg	1785.28	J/molxK	1176.49	Joback Method
cpg	1805.94	J/molxK	1224.29	Joback Method
cpg	1824.42	J/molxK	1272.08	Joback Method
cpg	1840.92	J/molxK	1319.87	Joback Method
cpg	1855.66	J/molxK	1367.66	Joback Method
dvisc	0.0001538	Paxs	597.14	Joback Method
dvisc	0.0000653	Paxs	677.77	Joback Method

dvisc	0.0000333	Paxs	758.40	Joback Method
dvisc	0.0000193	Paxs	839.02	Joback Method
dvisc	0.0000123	Paxs	919.65	Joback Method
dvisc	0.0000084	Paxs	1000.28	Joback Method
dvisc	0.0000061	Paxs	1080.91	Joback Method

## Sources

<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>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=U369751&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U369751&amp;Units=SI</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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