

# Diethylmalonic acid, heptadecyl hexyl ester

<b>Inchi:</b>	InChI=1S/C30H58O4/c1-5-9-11-13-14-15-16-17-18-19-20-21-22-23-25-27-34-29(32)30(7
<b>InchiKey:</b>	AFSSQUITELMSAX-UHFFFAOYSA-N
<b>Formula:</b>	C30H58O4
<b>SMILES:</b>	CCCCCCCCCCCCCCCCOC(=O)C(CC)(CC)C(=O)OCCCCC
<b>Mol. weight [g/mol]:</b>	482.78

## Physical Properties

Property code	Value	Unit	Source
gf	-263.28	kJ/mol	Joback Method
hf	-1160.88	kJ/mol	Joback Method
hfus	71.62	kJ/mol	Joback Method
hvap	99.39	kJ/mol	Joback Method
log10ws	-9.86		Crippen Method
logp	9.331		Crippen Method
mcvol	448.440	ml/mol	McGowan Method
pc	629.08	kPa	Joback Method
rinpol	3075.00		NIST Webbook
tb	1035.15	K	Joback Method
tc	1291.99	K	Joback Method
tf	574.60	K	Joback Method
vc	1.752	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1604.78	J/molxK	1035.15	Joback Method
cpg	1703.68	J/molxK	1249.18	Joback Method
cpg	1687.63	J/molxK	1206.38	Joback Method
cpg	1669.84	J/molxK	1163.57	Joback Method
cpg	1650.20	J/molxK	1120.76	Joback Method
cpg	1628.56	J/molxK	1077.96	Joback Method
cpg	1718.15	J/molxK	1291.99	Joback Method
dvisc	0.0000086	Paxs	1035.15	Joback Method
dvisc	0.0000118	Paxs	958.39	Joback Method

dvisc	0.0000171	Paxs	881.63	Joback Method
dvisc	0.0000267	Paxs	804.88	Joback Method
dvisc	0.0000457	Paxs	728.12	Joback Method
dvisc	0.0000890	Paxs	651.36	Joback Method
dvisc	0.0002068	Paxs	574.60	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=U369452&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U369452&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>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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