

# Diethylmalonic acid, decyl undecyl ester

<b>Inchi:</b>	InChI=1S/C28H54O4/c1-5-9-11-13-15-17-19-21-23-25-32-27(30)28(7-3,8-4)26(29)31-24
<b>InchiKey:</b>	MRFQSVZGXIKWPY-UHFFFAOYSA-N
<b>Formula:</b>	C28H54O4
<b>SMILES:</b>	CCCCCCCCCOC(=O)C(CC)(CC)C(=O)OCCCCCCCCC
<b>Mol. weight [g/mol]:</b>	454.73

## Physical Properties

Property code	Value	Unit	Source
gf	-280.12	kJ/mol	Joback Method
hf	-1119.60	kJ/mol	Joback Method
hfus	66.44	kJ/mol	Joback Method
hvap	94.94	kJ/mol	Joback Method
log10ws	-9.03		Crippen Method
logp	8.551		Crippen Method
mcvol	420.260	ml/mol	McGowan Method
pc	694.35	kPa	Joback Method
rinpol	2793.00		NIST Webbook
rinpol	2793.00		NIST Webbook
tb	989.39	K	Joback Method
tc	1222.65	K	Joback Method
tf	552.06	K	Joback Method
vc	1.641	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1474.13	J/molxK	989.39	Joback Method
cpg	1568.34	J/molxK	1183.77	Joback Method
cpg	1552.70	J/molxK	1144.89	Joback Method
cpg	1535.55	J/molxK	1106.02	Joback Method
cpg	1516.80	J/molxK	1067.14	Joback Method
cpg	1496.36	J/molxK	1028.27	Joback Method
cpg	1582.58	J/molxK	1222.65	Joback Method
dvisc	0.0000119	Paxs	989.39	Joback Method

dvisc	0.0000164	Paxs	916.50	Joback Method
dvisc	0.0000237	Paxs	843.61	Joback Method
dvisc	0.0000368	Paxs	770.72	Joback Method
dvisc	0.0000626	Paxs	697.84	Joback Method
dvisc	0.0001206	Paxs	624.95	Joback Method
dvisc	0.0002762	Paxs	552.06	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=U369501&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U369501&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.cheméo.com/doc/models/crippen_log10ws">https://www.cheméo.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>cp<sub>g</sub>:</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>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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