

# Diethylmalonic acid, hexyl 2-octyl ester

<b>Inchi:</b>	InChI=1S/C21H40O4/c1-6-10-12-14-16-18(5)25-20(23)21(8-3,9-4)19(22)24-17-15-13-11
<b>InchiKey:</b>	DTFITLMEXLXQMY-UHFFFAOYSA-N
<b>Formula:</b>	C21H40O4
<b>SMILES:</b>	CCCCCOC(=O)C(CC)(CC)C(=O)OC(C)CCCCC
<b>Mol. weight [g/mol]:</b>	356.54

## Physical Properties

Property code	Value	Unit	Source
gf	-341.50	kJ/mol	Joback Method
hf	-980.40	kJ/mol	Joback Method
hfus	44.78	kJ/mol	Joback Method
hvap	78.97	kJ/mol	Joback Method
log10ws	-6.21		Crippen Method
logp	5.818		Crippen Method
mcvol	321.630	ml/mol	McGowan Method
pc	1030.59	kPa	Joback Method
rinpol	2069.00		NIST Webbook
tb	828.79	K	Joback Method
tc	1018.11	K	Joback Method
tf	458.17	K	Joback Method
vc	1.242	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1031.48	J/molxK	828.79	Joback Method
cpg	1050.15	J/molxK	860.34	Joback Method
cpg	1067.69	J/molxK	891.90	Joback Method
cpg	1084.15	J/molxK	923.45	Joback Method
cpg	1099.56	J/molxK	955.00	Joback Method
cpg	1113.95	J/molxK	986.55	Joback Method
cpg	1127.36	J/molxK	1018.11	Joback Method
dvisc	0.0008434	Paxs	458.17	Joback Method
dvisc	0.0003582	Paxs	519.94	Joback Method

dvisc	0.0001825	Paxs	581.71	Joback Method
dvisc	0.0001058	Paxs	643.48	Joback Method
dvisc	0.0000675	Paxs	705.25	Joback Method
dvisc	0.0000463	Paxs	767.02	Joback Method
dvisc	0.0000336	Paxs	828.79	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=U369367&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U369367&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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