

# Diethylmalonic acid, hexyl octyl ester

<b>Inchi:</b>	InChI=1S/C21H40O4/c1-5-9-11-13-14-16-18-25-20(23)21(7-3,8-4)19(22)24-17-15-12-10
<b>InchiKey:</b>	IZZNIXUHIZGHRF-UHFFFAOYSA-N
<b>Formula:</b>	C21H40O4
<b>SMILES:</b>	CCCCCCCCOC(=O)C(CC)(CC)C(=O)OCCCCC
<b>Mol. weight [g/mol]:</b>	356.54

## Physical Properties

Property code	Value	Unit	Source
gf	-339.06	kJ/mol	Joback Method
hf	-975.12	kJ/mol	Joback Method
hfus	48.31	kJ/mol	Joback Method
hvap	79.36	kJ/mol	Joback Method
log10ws	-6.10		Crippen Method
logp	5.820		Crippen Method
mcvol	321.630	ml/mol	McGowan Method
pc	1025.31	kPa	Joback Method
rinpol	2157.00		NIST Webbook
tb	829.23	K	Joback Method
tc	1017.76	K	Joback Method
tf	473.17	K	Joback Method
vc	1.248	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1031.00	J/molxK	829.23	Joback Method
cpg	1049.60	J/molxK	860.65	Joback Method
cpg	1067.09	J/molxK	892.07	Joback Method
cpg	1083.51	J/molxK	923.49	Joback Method
cpg	1098.90	J/molxK	954.91	Joback Method
cpg	1113.29	J/molxK	986.33	Joback Method
cpg	1126.71	J/molxK	1017.76	Joback Method
dvisc	0.0007084	Paxs	473.17	Joback Method
dvisc	0.0003284	Paxs	532.51	Joback Method

dvisc	0.0001776	Paxs	591.86	Joback Method
dvisc	0.0001074	Paxs	651.20	Joback Method
dvisc	0.0000707	Paxs	710.54	Joback Method
dvisc	0.0000496	Paxs	769.89	Joback Method
dvisc	0.0000366	Paxs	829.23	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=U369443&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U369443&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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