

# Diethylmalonic acid, di(2-ethylhexyl) ester

<b>Inchi:</b>	InChI=1S/C23H44O4/c1-7-13-15-19(9-3)17-26-21(24)23(11-5,12-6)22(25)27-18-20(10-4
<b>InchiKey:</b>	YODPTQXQCQWQTN-UHFFFAOYSA-N
<b>Formula:</b>	C23H44O4
<b>SMILES:</b>	CCCCC(CC)COC(=O)C(CC)(CC)C(=O)OCC(CC)CCCC
<b>Mol. weight [g/mol]:</b>	384.59

## Physical Properties

Property code	Value	Unit	Source
gf	-327.10	kJ/mol	Joback Method
hf	-1026.96	kJ/mol	Joback Method
hfus	46.44	kJ/mol	Joback Method
hvap	83.03	kJ/mol	Joback Method
log10ws	-6.45		Crippen Method
logp	6.312		Crippen Method
mcvol	349.810	ml/mol	McGowan Method
pc	918.83	kPa	Joback Method
rinsol	2183.00		NIST Webbook
tb	874.11	K	Joback Method
tc	1070.79	K	Joback Method
tf	465.71	K	Joback Method
vc	1.349	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1155.68	J/molxK	874.11	Joback Method
cpg	1240.57	J/molxK	1038.01	Joback Method
cpg	1225.94	J/molxK	1005.23	Joback Method
cpg	1210.18	J/molxK	972.45	Joback Method
cpg	1193.24	J/molxK	939.67	Joback Method
cpg	1175.09	J/molxK	906.89	Joback Method
cpg	1254.12	J/molxK	1070.79	Joback Method
dvisc	0.0000224	Paxs	874.11	Joback Method
dvisc	0.0000315	Paxs	806.04	Joback Method

dvisc	0.0000472	Paxs	737.98	Joback Method
dvisc	0.0000767	Paxs	669.91	Joback Method
dvisc	0.0001392	Paxs	601.84	Joback Method
dvisc	0.0002941	Paxs	533.78	Joback Method
dvisc	0.0007729	Paxs	465.71	Joback Method

## Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=U369632&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U369632&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>
<b>McGowan Method:</b>	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</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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