

# Diethylmalonic acid, decyl hexyl ester

<b>Inchi:</b>	InChI=1S/C23H44O4/c1-5-9-11-13-14-15-16-18-20-27-22(25)23(7-3,8-4)21(24)26-19-17
<b>InchiKey:</b>	CHFCJYHIXJKWBL-UHFFFAOYSA-N
<b>Formula:</b>	C23H44O4
<b>SMILES:</b>	CCCCCCCCCOC(=O)C(CC)(CC)C(=O)OCCCCC
<b>Mol. weight [g/mol]:</b>	384.59

## Physical Properties

Property code	Value	Unit	Source
gf	-322.22	kJ/mol	Joback Method
hf	-1016.40	kJ/mol	Joback Method
hfus	53.49	kJ/mol	Joback Method
hvap	83.81	kJ/mol	Joback Method
log10ws	-6.93		Crippen Method
logp	6.600		Crippen Method
mvol	349.810	ml/mol	McGowan Method
pc	909.98	kPa	Joback Method
rinpol	2358.00		NIST Webbook
tb	874.99	K	Joback Method
tc	1071.31	K	Joback Method
tf	495.71	K	Joback Method
vc	1.361	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1154.79	J/molxK	874.99	Joback Method
cpg	1174.20	J/molxK	907.71	Joback Method
cpg	1192.37	J/molxK	940.43	Joback Method
cpg	1209.35	J/molxK	973.15	Joback Method
cpg	1225.18	J/molxK	1005.87	Joback Method
cpg	1239.91	J/molxK	1038.59	Joback Method
cpg	1253.57	J/molxK	1071.31	Joback Method
dvisc	0.0005484	Paxs	495.71	Joback Method
dvisc	0.0002494	Paxs	558.92	Joback Method

dvisc	0.0001331	Paxs	622.14	Joback Method
dvisc	0.0000798	Paxs	685.35	Joback Method
dvisc	0.0000521	Paxs	748.56	Joback Method
dvisc	0.0000364	Paxs	811.78	Joback Method
dvisc	0.0000268	Paxs	874.99	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=U369445&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U369445&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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