

# Diethylmalonic acid, hexyl 1-naphthyl ester

<b>Inchi:</b>	InChI=1S/C23H30O4/c1-4-7-8-11-17-26-21(24)23(5-2,6-3)22(25)27-20-16-12-14-18-13-9
<b>InchiKey:</b>	RYWONXSKKAGJFN-UHFFFAOYSA-N
<b>Formula:</b>	C23H30O4
<b>SMILES:</b>	CCCCCOC(=O)C(CC)(CC)C(=O)Oc1cccc2ccccc12
<b>Mol. weight [g/mol]:</b>	370.48

## Physical Properties

Property code	Value	Unit	Source
gf	-112.79	kJ/mol	Joback Method
hf	-600.27	kJ/mol	Joback Method
hfus	44.16	kJ/mol	Joback Method
hvap	88.39	kJ/mol	Joback Method
log10ws	-6.82		Crippen Method
logp	5.675		Crippen Method
mcvol	306.590	ml/mol	McGowan Method
pc	1318.48	kPa	Joback Method
rinsol	2622.00		NIST Webbook
tb	925.63	K	Joback Method
tc	1144.91	K	Joback Method
tf	567.35	K	Joback Method
vc	1.175	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	980.06	J/molxK	925.63	Joback Method
cpg	1046.57	J/molxK	1108.37	Joback Method
cpg	1035.11	J/molxK	1071.82	Joback Method
cpg	1022.82	J/molxK	1035.27	Joback Method
cpg	1009.60	J/molxK	998.72	Joback Method
cpg	995.38	J/molxK	962.18	Joback Method
cpg	1057.28	J/molxK	1144.91	Joback Method
dvisc	0.0000560	Paxs	925.63	Joback Method
dvisc	0.0000707	Paxs	865.92	Joback Method

dvisc	0.0000925	Paxs	806.20	Joback Method
dvisc	0.0001263	Paxs	746.49	Joback Method
dvisc	0.0001820	Paxs	686.78	Joback Method
dvisc	0.0002813	Paxs	627.06	Joback Method
dvisc	0.0004763	Paxs	567.35	Joback Method

## Sources

<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=U369870&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U369870&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>

## 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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