

# Diethylmalonic acid, ethyl 2-naphthyl ester

<b>Inchi:</b>	InChI=1S/C19H22O4/c1-4-19(5-2,17(20)22-6-3)18(21)23-16-12-11-14-9-7-8-10-15(14)13
<b>InchiKey:</b>	RPKXORQKGLZGBS-UHFFFAOYSA-N
<b>Formula:</b>	C19H22O4
<b>SMILES:</b>	CCOC(=O)C(CC)(CC)C(=O)Oc1ccc2ccccc2c1
<b>Mol. weight [g/mol]:</b>	314.38

## Physical Properties

Property code	Value	Unit	Source
gf	-146.47	kJ/mol	Joback Method
hf	-517.71	kJ/mol	Joback Method
hfus	33.80	kJ/mol	Joback Method
hvap	79.48	kJ/mol	Joback Method
log10ws	-5.14		Crippen Method
logp	4.115		Crippen Method
mvol	250.230	ml/mol	McGowan Method
pc	1780.34	kPa	Joback Method
rinpol	2314.00		NIST Webbook
rinpol	2314.00		NIST Webbook
tb	834.11	K	Joback Method
tc	1057.24	K	Joback Method
tf	522.27	K	Joback Method
vc	0.951	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	746.82	J/molxK	834.11	Joback Method
cpg	809.34	J/molxK	1020.05	Joback Method
cpg	798.71	J/molxK	982.86	Joback Method
cpg	787.23	J/molxK	945.67	Joback Method
cpg	774.80	J/molxK	908.49	Joback Method
cpg	761.35	J/molxK	871.30	Joback Method
cpg	819.17	J/molxK	1057.24	Joback Method
dvisc	0.0000973	Paxs	834.11	Joback Method

dvisc	0.0001212	Paxs	782.14	Joback Method
dvisc	0.0001558	Paxs	730.16	Joback Method
dvisc	0.0002082	Paxs	678.19	Joback Method
dvisc	0.0002919	Paxs	626.22	Joback Method
dvisc	0.0004351	Paxs	574.24	Joback Method
dvisc	0.0007020	Paxs	522.27	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=U369879&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U369879&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>cp<sub>g</sub>:</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>log<sub>10</sub>ws:</b>	Log <sub>10</sub> of Water solubility in mol/l
<b>logp:</b>	Octanol/Water partition coefficient
<b>m<sub>cvol</sub>:</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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