

# Dimethylmalonic acid, isobutyl 2-naphthylmethyl ester

Inchi:	InChI=1S/C20H24O4/c1-14(2)12-23-18(21)20(3,4)19(22)24-13-15-9-10-16-7-5-6-8-17(16)
InchiKey:	DMMCGFFOYNPJKA-UHFFFAOYSA-N
Formula:	C20H24O4
SMILES:	CC(C)COC(=O)C(C)(C)C(=O)OCc1ccc2ccccc2c1
Mol. weight [g/mol]:	328.40

## Physical Properties

Property code	Value	Unit	Source
gf	-140.49	kJ/mol	Joback Method
hf	-543.63	kJ/mol	Joback Method
hfus	32.86	kJ/mol	Joback Method
hvap	81.32	kJ/mol	Joback Method
log10ws	-5.16		Crippen Method
logp	4.108		Crippen Method
mcvol	264.320	ml/mol	McGowan Method
pc	1655.15	kPa	Joback Method
rinpol	2413.00		NIST Webbook
tb	856.55	K	Joback Method
tc	1080.56	K	Joback Method
tf	518.54	K	Joback Method
vc	1.000	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	804.48	J/molxK	856.55	Joback Method
cpg	868.50	J/molxK	1043.23	Joback Method
cpg	857.64	J/molxK	1005.89	Joback Method
cpg	845.88	J/molxK	968.56	Joback Method
cpg	833.15	J/molxK	931.22	Joback Method
cpg	819.38	J/molxK	893.89	Joback Method
cpg	878.55	J/molxK	1080.56	Joback Method
dvisc	0.0000779	Paxs	856.55	Joback Method
dvisc	0.0000988	Paxs	800.21	Joback Method

dvisc	0.0001299	Paxs	743.88	Joback Method
dvisc	0.0001787	Paxs	687.54	Joback Method
dvisc	0.0002602	Paxs	631.21	Joback Method
dvisc	0.0004077	Paxs	574.88	Joback Method
dvisc	0.0007043	Paxs	518.54	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=U363857&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U363857&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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