

# Diethylmalonic acid, 3-methylbenzyl octyl ester

Inchi:	InChI=1S/C23H36O4/c1-5-8-9-10-11-12-16-26-21(24)23(6-2,7-3)22(25)27-18-20-15-13-1
InchiKey:	XCXNFKMCHMFASS-UHFFFAOYSA-N
Formula:	C23H36O4
SMILES:	CCCCCCCCOC(=O)C(CC)(CC)C(=O)OCc1cccc(C)c1
Mol. weight [g/mol]:	376.53

## Physical Properties

Property code	Value	Unit	Source
gf	-219.44	kJ/mol	Joback Method
hf	-791.34	kJ/mol	Joback Method
hfus	47.14	kJ/mol	Joback Method
hvap	86.75	kJ/mol	Joback Method
log10ws	-6.59		Crippen Method
logp	5.748		Crippen Method
mcvol	326.050	ml/mol	McGowan Method
pc	1111.85	kPa	Joback Method
rinsol	2446.00		NIST Webbook
tb	906.65	K	Joback Method
tc	1114.81	K	Joback Method
tf	534.65	K	Joback Method
vc	1.252	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1058.41	J/molxK	906.65	Joback Method
cpg	1130.55	J/molxK	1080.12	Joback Method
cpg	1118.41	J/molxK	1045.42	Joback Method
cpg	1105.18	J/molxK	1010.73	Joback Method
cpg	1090.81	J/molxK	976.04	Joback Method
cpg	1075.23	J/molxK	941.34	Joback Method
cpg	1141.65	J/molxK	1114.81	Joback Method
dvisc	0.0000276	Paxs	906.65	Joback Method
dvisc	0.0000365	Paxs	844.65	Joback Method

dvisc	0.0000503	Paxs	782.65	Joback Method
dvisc	0.0000734	Paxs	720.65	Joback Method
dvisc	0.0001150	Paxs	658.65	Joback Method
dvisc	0.0001978	Paxs	596.65	Joback Method
dvisc	0.0003857	Paxs	534.65	Joback Method

## Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=U369310&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U369310&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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