

# Diethylmalonic acid, 2-methoxyethyl octyl ester

Inchi:	InChI=1S/C18H34O5/c1-5-8-9-10-11-12-13-22-16(19)18(6-2,7-3)17(20)23-15-14-21-4/h5
InchiKey:	PDRBXDZATXVFOL-UHFFFAOYSA-N
Formula:	C18H34O5
SMILES:	CCCCCCCCOC(=O)C(CC)(CC)C(=O)OCCOC
Mol. weight [g/mol]:	330.46

## Physical Properties

Property code	Value	Unit	Source
gf	-469.32	kJ/mol	Joback Method
hf	-1045.42	kJ/mol	Joback Method
hfus	41.72	kJ/mol	Joback Method
hvap	75.09	kJ/mol	Joback Method
log10ws	-3.93		Crippen Method
logp	3.886		Crippen Method
mcvol	285.230	ml/mol	McGowan Method
pc	1229.42	kPa	Joback Method
rinpol	1992.00		NIST Webbook
rinpol	1992.00		NIST Webbook
tb	783.01	K	Joback Method
tc	967.20	K	Joback Method
tf	461.59	K	Joback Method
vc	1.099	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	881.82	J/molxK	783.01	Joback Method
cpg	899.09	J/molxK	813.71	Joback Method
cpg	915.35	J/molxK	844.41	Joback Method
cpg	930.63	J/molxK	875.10	Joback Method
cpg	944.94	J/molxK	905.80	Joback Method
cpg	958.30	J/molxK	936.50	Joback Method
cpg	970.72	J/molxK	967.20	Joback Method
dvisc	0.0006811	Paxs	461.59	Joback Method

dvisc	0.0003384	Paxs	515.16	Joback Method
dvisc	0.0001918	Paxs	568.73	Joback Method
dvisc	0.0001199	Paxs	622.30	Joback Method
dvisc	0.0000808	Paxs	675.87	Joback Method
dvisc	0.0000576	Paxs	729.44	Joback Method
dvisc	0.0000431	Paxs	783.01	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=U370676&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U370676&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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