

# Diethylmalonic acid, butyl 5-methoxy-3-methylpentyl ester

Inchi:	InChI=1S/C18H34O5/c1-6-9-12-22-16(19)18(7-2,8-3)17(20)23-14-11-15(4)10-13-21-5/h1
InchiKey:	RRYXUNUEKODAGR-UHFFFAOYSA-N
Formula:	C18H34O5
SMILES:	CCCCOC(=O)C(CC)(CC)C(=O)OCCC(C)CCOC
Mol. weight [g/mol]:	330.46

## Physical Properties

Property code	Value	Unit	Source
gf	-471.76	kJ/mol	Joback Method
hf	-1050.70	kJ/mol	Joback Method
hfus	38.20	kJ/mol	Joback Method
hvap	74.70	kJ/mol	Joback Method
log10ws	-3.69		Crippen Method
logp	3.742		Crippen Method
mcvol	285.230	ml/mol	McGowan Method
pc	1236.35	kPa	Joback Method
rinpol	1935.00		NIST Webbook
rinpol	1935.00		NIST Webbook
tb	782.57	K	Joback Method
tc	968.21	K	Joback Method
tf	446.59	K	Joback Method
vc	1.093	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	882.32	J/molxK	782.57	Joback Method
cpg	959.26	J/molxK	937.27	Joback Method
cpg	945.86	J/molxK	906.33	Joback Method
cpg	931.48	J/molxK	875.39	Joback Method
cpg	916.11	J/molxK	844.45	Joback Method
cpg	899.73	J/molxK	813.51	Joback Method
cpg	971.71	J/molxK	968.21	Joback Method
dvisc	0.0000396	Paxs	782.57	Joback Method

dvisc	0.0000540	Paxs	726.57	Joback Method
dvisc	0.0000775	Paxs	670.58	Joback Method
dvisc	0.0001187	Paxs	614.58	Joback Method
dvisc	0.0001983	Paxs	558.58	Joback Method
dvisc	0.0003710	Paxs	502.59	Joback Method
dvisc	0.0008126	Paxs	446.59	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=U370764&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U370764&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.cheméo.com/doc/models/crippen_log10ws">https://www.cheméo.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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