

# Diethylmalonic acid, di(3-methylbutyl) ester

<b>Inchi:</b>	InChI=1S/C17H32O4/c1-7-17(8-2,15(18)20-11-9-13(3)4)16(19)21-12-10-14(5)6/h13-14H
<b>InchiKey:</b>	ZKJJCEMNIKSVGE-UHFFFAOYSA-N
<b>Formula:</b>	C17H32O4
<b>SMILES:</b>	CCC(CC)(C(=O)OCCC(C)C)C(=O)OCCC(C)C
<b>Mol. weight [g/mol]:</b>	300.43

## Physical Properties

Property code	Value	Unit	Source
gf	-377.62	kJ/mol	Joback Method
hf	-903.12	kJ/mol	Joback Method
hfus	30.90	kJ/mol	Joback Method
hvap	69.68	kJ/mol	Joback Method
log10ws	-3.94		Crippen Method
logp	3.971		Crippen Method
mcvol	265.270	ml/mol	McGowan Method
pc	1348.67	kPa	Joback Method
rinpol	1676.00		NIST Webbook
rinpol	1676.00		NIST Webbook
tb	736.83	K	Joback Method
tc	922.80	K	Joback Method
tf	398.09	K	Joback Method
vc	1.012	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	793.82	J/molxK	736.83	Joback Method
cpg	811.45	J/molxK	767.82	Joback Method
cpg	828.10	J/molxK	798.82	Joback Method
cpg	843.79	J/molxK	829.81	Joback Method
cpg	858.54	J/molxK	860.81	Joback Method
cpg	872.39	J/molxK	891.80	Joback Method
cpg	885.36	J/molxK	922.80	Joback Method
dvisc	0.0017460	Paxs	398.09	Joback Method

dvisc	0.0006925	Paxs	454.55	Joback Method
dvisc	0.0003369	Paxs	511.00	Joback Method
dvisc	0.0001892	Paxs	567.46	Joback Method
dvisc	0.0001179	Paxs	623.92	Joback Method
dvisc	0.0000795	Paxs	680.37	Joback Method
dvisc	0.0000570	Paxs	736.83	Joback Method

## Sources

<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>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=U369398&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U369398&amp;Units=SI</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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