

# Dimethylmalonic acid, ethyl isobutyl ester

<b>Inchi:</b>	InChI=1S/C11H20O4/c1-6-14-9(12)11(4,5)10(13)15-7-8(2)3/h8H,6-7H2,1-5H3
<b>InchiKey:</b>	PDJZBTJFISLLLN-UHFFFAOYSA-N
<b>Formula:</b>	C11H20O4
<b>SMILES:</b>	CCOC(=O)C(C)(C)C(=O)OCC(C)C
<b>Mol. weight [g/mol]:</b>	216.27

## Physical Properties

Property code	Value	Unit	Source
gf	-425.70	kJ/mol	Joback Method
hf	-774.00	kJ/mol	Joback Method
hfus	18.88	kJ/mol	Joback Method
hvap	56.71	kJ/mol	Joback Method
log10ws	-1.67		Crippen Method
logp	1.775		Crippen Method
mcvol	180.730	ml/mol	McGowan Method
pc	2153.30	kPa	Joback Method
rinpol	1235.00		NIST Webbook
tb	599.99	K	Joback Method
tc	791.04	K	Joback Method
tf	345.47	K	Joback Method
vc	0.682	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	468.59	J/molxK	599.99	Joback Method
cpg	483.45	J/molxK	631.83	Joback Method
cpg	497.56	J/molxK	663.67	Joback Method
cpg	510.92	J/molxK	695.51	Joback Method
cpg	523.56	J/molxK	727.36	Joback Method
cpg	535.49	J/molxK	759.20	Joback Method
cpg	546.72	J/molxK	791.04	Joback Method
dvisc	0.0025750	Paxs	345.47	Joback Method
dvisc	0.0012195	Paxs	387.89	Joback Method

dvisc	0.0006692	Paxs	430.31	Joback Method
dvisc	0.0004090	Paxs	472.73	Joback Method
dvisc	0.0002711	Paxs	515.15	Joback Method
dvisc	0.0001913	Paxs	557.57	Joback Method
dvisc	0.0001418	Paxs	599.99	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=U361649&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U361649&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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