

# Diethylmalonic acid, isobutyl propyl ester

<b>Inchi:</b>	InChI=1S/C14H26O4/c1-6-9-17-12(15)14(7-2,8-3)13(16)18-10-11(4)5/h11H,6-10H2,1-5H
<b>InchiKey:</b>	IFFPZINUGAWSLL-UHFFFAOYSA-N
<b>Formula:</b>	C14H26O4
<b>SMILES:</b>	CCCOC(=O)C(CC)(CC)C(=O)OCC(C)C
<b>Mol. weight [g/mol]:</b>	258.35

## Physical Properties

Property code	Value	Unit	Source
gf	-400.44	kJ/mol	Joback Method
hf	-835.92	kJ/mol	Joback Method
hfus	26.65	kJ/mol	Joback Method
hvap	63.39	kJ/mol	Joback Method
log10ws	-2.92		Crippen Method
logp	2.945		Crippen Method
mcvol	223.000	ml/mol	McGowan Method
pc	1675.53	kPa	Joback Method
rinpol	1466.00		NIST Webbook
tb	668.63	K	Joback Method
tc	854.31	K	Joback Method
tf	379.28	K	Joback Method
vc	0.851	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	625.23	J/molxK	668.63	Joback Method
cpg	641.58	J/molxK	699.58	Joback Method
cpg	657.08	J/molxK	730.52	Joback Method
cpg	671.74	J/molxK	761.47	Joback Method
cpg	685.59	J/molxK	792.42	Joback Method
cpg	698.63	J/molxK	823.36	Joback Method
cpg	710.90	J/molxK	854.31	Joback Method
dvisc	0.0019390	Paxs	379.28	Joback Method
dvisc	0.0008833	Paxs	427.50	Joback Method

dvisc	0.0004719	Paxs	475.73	Joback Method
dvisc	0.0002830	Paxs	523.96	Joback Method
dvisc	0.0001849	Paxs	572.18	Joback Method
dvisc	0.0001291	Paxs	620.40	Joback Method
dvisc	0.0000950	Paxs	668.63	Joback Method

## Sources

<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=U369420&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U369420&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307l">http://pubs.acs.org/doi/abs/10.1021/ci990307l</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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