

# DL-3-Aminoisobutyric acid, N-dimethylaminomethylene-, methyl ester

**Inchi:** InChI=1S/C8H16N2O2/c1-7(8(11)12-4)5-9-6-10(2)3/h6-7H,5H2,1-4H3  
**InchiKey:** LNSOEGTZANBNKJ-UHFFFAOYSA-N  
**Formula:** C8H16N2O2  
**SMILES:** COC(=O)C(C)CN=CN(C)C  
**Mol. weight [g/mol]:** 172.22

## Physical Properties

Property code	Value	Unit	Source
hf	-308.78	kJ/mol	Joback Method
hvap	47.53	kJ/mol	Joback Method
log10ws	-0.02		Crippen Method
logp	0.385		Crippen Method
mcvol	146.680	ml/mol	McGowan Method
pc	2405.28	kPa	Joback Method
rinpol	1243.00		NIST Webbook
rinpol	1243.00		NIST Webbook
tb	547.41	K	Joback Method
tc	741.73	K	Joback Method

## Sources

**Crippen Method:** [https://www.chemeo.com/doc/models/crippen\\_log10ws](https://www.chemeo.com/doc/models/crippen_log10ws)  
**Joback Method:** [https://en.wikipedia.org/wiki/Joback\\_method](https://en.wikipedia.org/wiki/Joback_method)  
**McGowan Method:** <http://link.springer.com/article/10.1007/BF02311772>  
**NIST Webbook:** <http://webbook.nist.gov/cgi/cbook.cgi?ID=U375503&Units=SI>  
**Crippen Method:** <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

## Legend

**hf:** Enthalpy of formation at standard conditions  
**hvap:** 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

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