

# 5-Aminovaleric acid, N-dimethylaminomethylene-, methyl ester

**Inchi:** InChI=1S/C9H18N2O2/c1-11(2)8-10-7-5-4-6-9(12)13-3/h8H,4-7H2,1-3H3  
**InchiKey:** YRGMVGZUSCSTSE-UHFFFAOYSA-N  
**Formula:** C9H18N2O2  
**SMILES:** COC(=O)CCCCN=CN(C)C  
**Mol. weight [g/mol]:** 186.25

## Physical Properties

Property code	Value	Unit	Source
hf	-324.14	kJ/mol	Joback Method
hvap	50.14	kJ/mol	Joback Method
log10ws	-0.68		Crippen Method
logp	0.920		Crippen Method
mcvol	160.770	ml/mol	McGowan Method
pc	2177.49	kPa	Joback Method
rinpol	1412.00		NIST Webbook
rinpol	1412.00		NIST Webbook
tb	570.73	K	Joback Method
tc	758.91	K	Joback Method

## Sources

**NIST Webbook:** <http://webbook.nist.gov/cgi/cbook.cgi?ID=U375797&Units=SI>  
**Crippen Method:** <http://pubs.acs.org/doi/abs/10.1021/ci990307l>  
**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>

## 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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