

# 1-Aminocyclopropanecarboxylic acid, N-dimethylaminomethylene-, butyl ester

<b>Inchi:</b>	InChI=1S/C11H20N2O2/c1-4-5-8-15-10(14)11(6-7-11)12-9-13(2)3/h9H,4-8H2,1-3H3
<b>InchiKey:</b>	WCBUMINPAZPOQF-UHFFFAOYSA-N
<b>Formula:</b>	C11H20N2O2
<b>SMILES:</b>	CCCCOC(=O)C1(N=CN(C)C)CC1
<b>Mol. weight [g/mol]:</b>	212.29

## Physical Properties

Property code	Value	Unit	Source
hf	-277.38	kJ/mol	Joback Method
hvap	53.36	kJ/mol	Joback Method
log10ws	-1.53		Crippen Method
logp	1.452		Crippen Method
mcvol	178.090	ml/mol	McGowan Method
pc	2143.35	kPa	Joback Method
rinpol	1540.00		NIST Webbook
rinpol	1540.00		NIST Webbook
tb	623.47	K	Joback Method
tc	826.11	K	Joback Method

## Sources

<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=U375509&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U375509&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307I">http://pubs.acs.org/doi/abs/10.1021/ci990307I</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>

## Legend

<b>hf:</b>	Enthalpy of formation 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

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