

# L-2-Aminobutyric acid, N-dimethylaminomethylene-, butyl ester

**Inchi:** InChI=1S/C11H22N2O2/c1-5-7-8-15-11(14)10(6-2)12-9-13(3)4/h9-10H,5-8H2,1-4H3  
**InchiKey:** LJNUSTICJXXZEL-UHFFFAOYSA-N  
**Formula:** C11H22N2O2  
**SMILES:** CCCOC(=O)C(CC)N=CN(C)C  
**Mol. weight [g/mol]:** 214.30

## Physical Properties

Property code	Value	Unit	Source
hf	-370.70	kJ/mol	Joback Method
hvap	54.20	kJ/mol	Joback Method
log10ws	-1.63		Crippen Method
logp	1.698		Crippen Method
mcvol	188.950	ml/mol	McGowan Method
pc	1846.75	kPa	Joback Method
rinpol	1480.00		NIST Webbook
tb	616.05	K	Joback Method
tc	803.58	K	Joback Method

## Sources

**NIST Webbook:** <http://webbook.nist.gov/cgi/cbook.cgi?ID=U375525&Units=SI>  
**Crippen Method:** <http://pubs.acs.org/doi/abs/10.1021/ci9903071>  
**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  
**log10ws:** 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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