

# 1-Aminocyclopentanecarboxylic acid, N-(isobutoxycarbonyl)-, tridecyl ester

**Inchi:** InChI=1S/C24H45NO4/c1-4-5-6-7-8-9-10-11-12-13-16-19-28-22(26)24(17-14-15-18-24)2  
**InchiKey:** ISPAUEUFXMSKDS-UHFFFAOYSA-N  
**Formula:** C24H45NO4  
**SMILES:** CCCCCCCCCCCCCOC(=O)C1(N=C(O)OCC(C)C)CCCC1  
**Mol. weight [g/mol]:** 411.62

## Physical Properties

Property code	Value	Unit	Source
hf	-925.07	kJ/mol	Joback Method
hvap	99.37	kJ/mol	Joback Method
log10ws	-7.06		Crippen Method
logp	6.740		Crippen Method
mcvol	363.020	ml/mol	McGowan Method
pc	936.35	kPa	Joback Method
rinpol	2815.00		NIST Webbook
tb	1031.05	K	Joback Method
tc	1266.02	K	Joback Method

## Sources

**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>  
**NIST Webbook:** <http://webbook.nist.gov/cgi/cbook.cgi?ID=U392510&Units=SI>

## 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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