

# N-Carboxyethylangustifoline

**Inchi:** InChI=1S/C17H26N2O3/c1-3-5-15-14-8-12(11-19(15)17(21)22-4-2)10-18-7-6-13(20)9-16  
**InchiKey:** IKBYKUDNGCYJDC-UHFFFAOYSA-N  
**Formula:** C17H26N2O3  
**SMILES:** C=CCC1C2CC(CN3CCC(=O)CC23)CN1C(=O)OCC  
**Mol. weight [g/mol]:** 306.40

## Physical Properties

Property code	Value	Unit	Source
log10ws	-2.48		Crippen Method
logp	2.073		Crippen Method
mcvol	242.480	ml/mol	McGowan Method
rinpole	2305.00		NIST Webbook
rinpole	2305.00		NIST Webbook

## Sources

**McGowan Method:** <http://link.springer.com/article/10.1007/BF02311772>  
**NIST Webbook:** <http://webbook.nist.gov/cgi/cbook.cgi?ID=R264290&Units=SI>  
**Crippen Method:** <http://pubs.acs.org/doi/abs/10.1021/ci9903071>  
**Crippen Method:** [https://www.cheméo.com/doc/models/crippen\\_log10ws](https://www.cheméo.com/doc/models/crippen_log10ws)

## Legend

**log10ws:** Log10 of Water solubility in mol/l  
**logp:** Octanol/Water partition coefficient  
**mcvol:** McGowan's characteristic volume  
**rinpole:** Non-polar retention indices

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