N-Methylangustifoline

Inchi: InChI=1S/C15H24N2O/c1-3-4-14-13-7-11(9-16(14)2)10-17-6-5-12(18)8-15(13)17/h3,11,1
InchiKey: QQUUXSNDZUAQQT-UHFFFAOYSA-N
Formula: C15H24N2O
SMILES: C=CCC1C2CC(CN1C)CN1CCC(=O)CC21
Mol. weight [g/mol]: 248.36

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.80		Crippen Method
logp	1.546		Crippen Method
mcvol	206.860	ml/mol	McGowan Method
rinpol	2073.00		NIST Webbook
rinpol	2050.00		NIST Webbook

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R109183&Units=SI

Legend

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

Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.