N-Methylalbine

Inchi: InChI=1S/C15H22N2O/c1-3-4-14-13-7-11(9-16(14)2)10-17-6-5-12(18)8-15(13)17/h3,5-6,
InchiKey: HPMYEIHKHIJZJW-AXVKAWJUSA-N
Formula: C15H22N2O
SMILES: C=CCC1C2CC(CN1C)CN1C=CC(=O)CC21
Mol. weight [g/mol]: 246.35

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.15		Crippen Method
logp	1.670		Crippen Method
mcvol	202.560	ml/mol	McGowan Method
rinpol	2215.00		NIST Webbook
rinpol	2220.00		NIST Webbook
rinpol	2215.00		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=R308508&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