

Adamantane, 1-(4-morpholyI)

Inchi: InChI=1S/C14H23NO/c1-3-16-4-2-15(1)14-8-11-5-12(9-14)7-13(6-11)10-14/h11-13H,1-14H
InchiKey: PHYMGSYTSU ESSU-UHFFFAOYSA-N
Formula: C14H23NO
SMILES: C1CN(C23CC4CC(CC(C4)C2)C3)CCO1
Mol. weight [g/mol]: 221.34

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.31		Crippen Method
logp	2.287		Crippen Method
mcvol	180.530	ml/mol	McGowan Method
rinpol	1821.00		NIST Webbook
rinpol	1821.00		NIST Webbook

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.cheméo.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=R44423&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

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