

Adamantane, 2-(1-pyrrolyl)

Inchi: InChI=1S/C14H19N/c1-2-4-15(3-1)14-12-6-10-5-11(8-12)9-13(14)7-10/h1-4,10-14H,5-9H
InchiKey: NKAKMZFOLXTWSK-UHFFFAOYSA-N
Formula: C14H19N
SMILES: c1ccn(C2C3CC4CC(C3)CC2C4)c1
Mol. weight [g/mol]: 201.31

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.76		Crippen Method
logp	3.485		Crippen Method
mcvol	166.060	ml/mol	McGowan Method
rinpol	1658.00		NIST Webbook

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
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=R44441&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

Latest version available from:

<https://www.chemeo.com/cid/25-054-4/Adamantane-2-1-pyrrolyl.pdf>

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