

Adamantane, 2-(1-piperazinylyl)

Inchi: InChI=1S/C15H25N/c1-2-4-16(5-3-1)15-13-7-11-6-12(9-13)10-14(15)8-11/h11-15H,1-10H
InchiKey: JLODQGUVAJFVBE-UHFFFAOYSA-N
Formula: C15H25N
SMILES: C1CCN(C2C3CC4CC(C3)CC2C4)CC1
Mol. weight [g/mol]: 219.37

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.40		Crippen Method
logp	3.297		Crippen Method
mcvol	188.750	ml/mol	McGowan Method
rinpola	1849.00		NIST Webbook

Sources

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R44437&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

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

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<https://www.chemeo.com/cid/43-425-2/Adamantane-2-1-piperazinylyl.pdf>

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