

1-Adamantanecarboxylic acid, morpholide

Inchi: InChI=1S/C15H23NO2/c17-14(16-1-3-18-4-2-16)15-8-11-5-12(9-15)7-13(6-11)10-15/h11
InchiKey: CHKCQWNXMJAHPZ-UHFFFAOYSA-N
Formula: C15H23NO2
SMILES: O=C(N1CCOCC1)C12CC3CC(CC(C3)C1)C2
Mol. weight [g/mol]: 249.35

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.15		Crippen Method
logp	2.062		Crippen Method
mcvol	196.190	ml/mol	McGowan Method
rinpol	2098.00		NIST Webbook
rinpol	2098.00		NIST Webbook

Sources

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=U307463&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>

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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