

N-DesmethyImirtazapine

Inchi: InChI=1S/C16H17N3/c1-2-6-14-12(4-1)10-13-5-3-7-18-16(13)19-9-8-17-11-15(14)19/h1-
InchiKey: FGLAMNFOHWVQOH-UHFFFAOYSA-N
Formula: C16H17N3
SMILES: c1ccc2c(c1)Cc1cccnc1N1CCNCC21
Mol. weight [g/mol]: 251.33
CAS: 61337-68-6

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.49		Crippen Method
logp	2.137		Crippen Method
mcvol	197.000	ml/mol	McGowan Method
rinpola	2375.80		NIST Webbook
rinpola	2375.80		NIST Webbook

Sources

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C61337686&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
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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