

11,12-seco-Multiflorine

Inchi: InChI=1S/C15H24N2O/c1-2-3-5-16-9-12-7-13(11-16)15-8-14(18)4-6-17(15)10-12/h4,6,12
InchiKey: QLDWYEWYOYNNAMI-GUTXKFCHSA-N
Formula: C15H24N2O
SMILES: CCCC1CC2CC(C1)C1CC(=O)C=CN1C2
Mol. weight [g/mol]: 248.36

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.18		Crippen Method
logp	1.895		Crippen Method
mcvol	206.860	ml/mol	McGowan Method
rinpole	2225.00		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R577749&Units=SI>
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>

Legend

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

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