

Multiflorine

Inchi: InChI=1S/C15H22N2O/c18-13-4-6-17-9-11-7-12(15(17)8-13)10-16-5-2-1-3-14(11)16/h4,6,10,12,14,15,17,18
InchiKey: HQSKZPOVBDNEGN-UHFFFAOYSA-N
Formula: C15H22N2O
SMILES: O=C1C=CN2CC3CC(CN4CCCCC34)C2C1
Mol. weight [g/mol]: 246.35
CAS: 529-80-6

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.19		Crippen Method
logp	1.648		Crippen Method
mcvol	196.000	ml/mol	McGowan Method
rinpol	2310.00		NIST Webbook
rinpol	2320.00		NIST Webbook
rinpol	2310.00		NIST Webbook
rinpol	2320.00		NIST Webbook
rinpol	2320.00		NIST Webbook
rinpol	2310.00		NIST Webbook
rinpol	2310.00		NIST Webbook

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>
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=C529806&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/61-465-8/Multiflorine.pdf>

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