

Multiflorine

Inchi: InChI=1S/C15H24N2O/c18-13-4-6-17-9-11-7-12(15(17)8-13)10-16-5-2-1-3-14(11)16/h11
InchiKey: RYLSVBDVGRSVHE-UHFFFAOYSA-N
Formula: C15H24N2O
SMILES: O=C1CCN2CC3CC(CN4CCCCC34)C2C1
Mol. weight [g/mol]: 248.36

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.84		Crippen Method
logp	1.524		Crippen Method
mcvol	200.300	ml/mol	McGowan Method
rinsol	2310.00		NIST Webbook
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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=R598751&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

Legend

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

Latest version available from:

<https://www.chemeo.com/cid/77-052-9/Multiflorine.pdf>

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