

Dihydromultifiorine

Inchi: InChI=1S/C15H26N2O/c18-13-4-6-17-9-11-7-12(15(17)8-13)10-16-5-2-1-3-14(11)16/h11
InchiKey: MMXKVQSOWVEFOB-UHFFFAOYSA-N
Formula: C15H26N2O
SMILES: OC1CCN2CC3CC(CN4CCCCC34)C2C1
Mol. weight [g/mol]: 250.38

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.94		Crippen Method
logp	1.316		Crippen Method
mcvol	204.600	ml/mol	McGowan Method
rinpol	2100.00		NIST Webbook
rinpol	2100.00		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=R264176&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

Latest version available from:

<https://www.chemeo.com/cid/49-113-2/Dihydromultifiorine.pdf>

Generated by Cheméo on 2024-04-25 21:59:10.99219766 +0000 UTC m=+16371599.912774981.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.