5,6-Dehydromultiflorine

Inchi: InChI=1S/C15H20N2O/c18-13-4-6-17-9-11-7-12(15(17)8-13)10-16-5-2-1-3-14(11)16/h4,6
InchiKey: SJRGHHOFXSLZOB-ORHYLEIMSA-N
Formula: C15H20N2O
SMILES: O=c1ccn2c(c1)C1CC(C2)C2CCCCN2C1
Mol. weight [g/mol]: 244.33

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.56		Crippen Method
logp	1.820		Crippen Method
mcvol	191.700	ml/mol	McGowan Method
rinpol	2110.00		NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R557072&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
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
rinpol: Non-polar retention indices