

Adeptolon, N-desethyl, acetylated

Inchi: InChI=1S/C16H18BrN3O/c1-13(21)19(2)11-12-20(16-5-3-4-10-18-16)15-8-6-14(17)7-9-1
InchiKey: ZRQIBQJSGUCEDN-UHFFFAOYSA-N
Formula: C16H18BrN3O
SMILES: CC(=O)N(C)CCN(c1ccc(Br)cc1)c1cccn1
Mol. weight [g/mol]: 348.24

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.12		Crippen Method
logp	3.460		Crippen Method
mcvol	237.790	ml/mol	McGowan Method
rinpol	2470.00		NIST Webbook

Sources

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>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R535998&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/51-712-4/Adeptolon-N-desethyl-acetylated.pdf>

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