

Adeptolon, N-desethyl-hydroxy, acetylated

Inchi: InChI=1S/C18H20BrN3O3/c1-13(23)21(3)10-11-22(16-6-4-15(19)5-7-16)18-9-8-17(12-20)
InchiKey: LRVZAZRNQMPQMJ-UHFFFAOYSA-N
Formula: C18H20BrN3O3
SMILES: CC(=O)Oc1ccc(N(CCN(C)C(C)=O)c2ccc(Br)cc2)nc1
Mol. weight [g/mol]: 406.27

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.44		Crippen Method
logp	3.386		Crippen Method
mcvol	273.410	ml/mol	McGowan Method
rinpol	3010.00		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=R536000&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

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<https://www.chemeo.com/cid/17-977-9/Adeptolon-N-desethyl-hydroxy-acetylated.pdf>

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