

Adeptolon, hydroxy, acetylated

Inchi: InChI=1S/C18H22BrN3O2/c1-4-21(3)11-12-22(16-7-5-15(19)6-8-16)18-10-9-17(13-20-18)
InchiKey: KLTREHAGUDIVQM-UHFFFAOYSA-N
Formula: C18H22BrN3O2
SMILES: CCN(C)CCN(c1ccc(Br)cc1)c1ccc(OC(C)=O)cn1
Mol. weight [g/mol]: 392.29

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.66		Crippen Method
logp	3.859		Crippen Method
mcvol	271.840	ml/mol	McGowan Method
rinpol	2780.00		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R535963&Units=SI>
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>

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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