Noradeptolon, hydroxy, acetylated

Inchi: InChI=1S/C19H22BrN3O3/c1-14(24)22(3)10-11-23(13-16-4-6-17(20)7-5-16)19-12-18(8-9
InchiKey: BKYXWWWDVSJHJP-UHFFFAOYSA-N
Formula: C19H22BrN3O3
SMILES: CC(=O)Oc1ccnc(N(CCN(C)C(C)=O)Cc2ccc(Br)cc2)c1
Mol. weight [g/mol]: 420.30

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.75		Crippen Method
logp	3.254		Crippen Method
mcvol	287.500	ml/mol	McGowan Method
rinpol	3030.00		NIST Webbook
rinpol	3030.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R536604&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
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

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