

Noradephton, acetylated

Inchi:	InChI=1S/C17H20BrN3O/c1-14(22)20(2)11-12-21(17-5-3-4-10-19-17)13-15-6-8-16(18)9-
InchiKey:	VABYWFIUOMB BTBI-UHFFFAOYSA-N
Formula:	C17H20BrN3O
SMILES:	CC(=O)N(C)CCN(Cc1ccc(Br)cc1)c1cccn1
Mol. weight [g/mol]:	362.26

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.44		Crippen Method
logp	3.329		Crippen Method
mcvol	251.880	ml/mol	McGowan Method
rinpol	2530.00		NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R536595&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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

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<https://www.chemeo.com/cid/56-675-1/Noradephton-acetylated.pdf>

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