

bromazepam-N(Py)-oxide

Inchi:	InChI=1S/C14H10BrN3O2/c15-9-4-5-11-10(7-9)14(16-8-13(19)17-11)12-3-1-2-6-18(12)2
InchiKey:	UXBHJGIEDLZVCU-UHFFFAOYSA-N
Formula:	C14H10BrN3O2
SMILES:	O=C1CN=C(c2cccc[n+]2[O-])c2cc(Br)ccc2N1
Mol. weight [g/mol]:	332.15

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.63		Crippen Method
logp	1.872		Crippen Method
mcvol	200.320	ml/mol	McGowan Method
rinpole	2650.00		NIST Webbook

Sources

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=R248496&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpole:	Non-polar retention indices

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