

Bromazepam-3-hydroxy

Other names:	7-Bromo-3-hydroxy-5-(2-pyridinyl)-1,3-dihydro-2H-1,4-benzodiazepin-2-one 3-Hydroxybromazepam 2H-1,4-Benzodiazepin-2-one, 7-bromo-1,3-dihydro-3-hydroxy-5-(2-pyridinyl)-
Inchi:	InChI=1S/C14H10BrN3O2/c15-8-4-5-10-9(7-8)12(11-3-1-2-6-16-11)18-14(20)13(19)17-1
InchiKey:	URRUSNGCYBXNLO-UHFFFAOYSA-N
Formula:	C14H10BrN3O2
SMILES:	O=C1Nc2ccc(Br)cc2C(c2ccccc2)=NC1O
Mol. weight [g/mol]:	332.15
CAS:	13132-73-5

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.74		Crippen Method
logp	1.952		Crippen Method
mcvol	200.320	ml/mol	McGowan Method
rinpol	2540.00		NIST Webbook
rinpol	2568.00		NIST Webbook
rinpol	2540.00		NIST Webbook
rinpol	2555.00		NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C13132735&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

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