

Bromazepam M (3-hydroxy-), hydrolysis, acetylated

Inchi: InChI=1S/C14H11BrN2O2/c1-9(18)17-12-6-5-10(15)8-11(12)14(19)13-4-2-3-7-16-13/h2-
InchiKey: GROKCASTURVYLG-UHFFFAOYSA-N
Formula: C14H11BrN2O2
SMILES: CC(=O)Nc1ccc(Br)cc1C(=O)c1cccn1
Mol. weight [g/mol]: 319.15

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.56		Crippen Method
logp	3.033		Crippen Method
mcvol	201.200	ml/mol	McGowan Method
rinpol	2490.00		NIST Webbook
rinpol	2490.00		NIST Webbook
rinpol	2490.00		NIST Webbook

Sources

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>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R312775&Units=SI>

Legend

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

Latest version available from:

<https://www.chemeo.com/cid/67-672-2/Bromazepam-M-3-hydroxy-hydrolysis-acetylated.pdf>

Generated by Cheméo on 2024-04-30 15:33:03.105239879 +0000 UTC m=+16780432.025817194.

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