

Brotizolam, M (hydroxy-), acetylated

Inchi: InChI=1S/C17H12BrClN4O2S/c1-8-21-22-15-16(25-9(2)24)20-14(10-5-3-4-6-12(10)19)1
InchiKey: IRHPIDZMALJHFL-UHFFFAOYSA-N
Formula: C17H12BrClN4O2S
SMILES: CC(=O)OC1N=C(c2ccccc2Cl)c2cc(Br)sc2-n2c(C)nnc21
Mol. weight [g/mol]: 451.73

Physical Properties

Property code	Value	Unit	Source
log10ws	-7.04		Crippen Method
logp	4.466		Crippen Method
mcvol	266.000	ml/mol	McGowan Method
rinpol	3140.00		NIST Webbook
rinpol	3140.00		NIST Webbook

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.cheméo.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=R312780&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

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