

Brotizolam, M (hydroxy-), acetylated

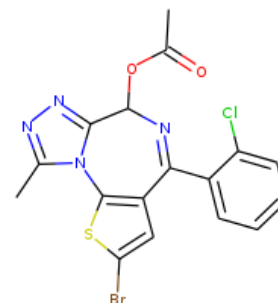
InChI: InChI=1S/C17H12BrClN4O2S/c1-8-21-22-15-16(25-9(2)24)20-14(10-5-3-4-6-12(10)19)11-7-13(18)26-17(11)23(8)15/h3-7,16H,1-2H3

InChI Key: IRHPIDZMALJHFL-UHFFFAOYSA-N

Formula: C₁₇H₁₂BrClN₄O₂S

SMILES: CC(=O)OC1N=C(c2ccccc2Cl)c2cc(Br)sc2-n2c(C)nnc21

Molecular Weight: 451.73



Physical Properties

Property	Value	Unit	Source
$\log P_{\text{oct/wat}}$	4.47		Crippen Method

Sources

NIST Webbook: [http://webbook.nist.gov/cgi/inchi/InChI=1S/C17H12BrClN4O2S/c1-8-21-22-15-16\(25-9\(2\)24\)20-14\(10-5-3-4-6-12\(10\)19\)11-7-13\(18\)26-17\(11\)23\(8\)15/h3-7,16H,1-2H3](http://webbook.nist.gov/cgi/inchi/InChI=1S/C17H12BrClN4O2S/c1-8-21-22-15-16(25-9(2)24)20-14(10-5-3-4-6-12(10)19)11-7-13(18)26-17(11)23(8)15/h3-7,16H,1-2H3)

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

Legend

$\log P_{\text{oct/wat}}$: Octanol/Water partition coefficient .

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