

Brotizolam

Other names:	6H-Thieno[3,2-f][1,2,4]triazolo[4,3-a][1,4]diazepine, 2-bromo-4-(2-chlorophenyl)-9-methyl- 2-Bromo-4-(2-chlorophenyl)-9-methyl-6H-thieno(3,2-f)(1,2,4)triazolo(4,3-a)(1,4)diazepine Lendormin WE 941 WE 941-BS 2-Bromo-4-(o-chlorophenyl)-9-methyl-6H-thieno[3,2-f]-s-triazolo[4,3-a]-[1,4]diazepine Lendorm Mederantil Sintonal
Inchi:	InChI=1S/C15H10BrClN4S/c1-8-19-20-13-7-18-14(9-4-2-3-5-11(9)17)10-6-12(16)22-15(1
InchiKey:	UMSGKTJDUHERQW-UHFFFAOYSA-N
Formula:	C15H10BrClN4S
SMILES:	Cc1nnc2n1-c1sc(Br)cc1C(c1ccccc1Cl)=NC2
Mol. weight [g/mol]:	393.69
CAS:	57801-81-7

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.88		Crippen Method
logp	4.404		Crippen Method
mcvol	230.380	ml/mol	McGowan Method
rinpol	3090.00		NIST Webbook

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C57801817&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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