

Lormetazepam

Other names:	2H-1,4-Benzodiazepin-2-one, 7-chloro-5-(2-chlorophenyl)-1,3-dihydro-3-hydroxy-1-methyl- 2H-1,4-Benzodiazepin-2-one, 1,3-dihydro-7-chloro-5-(o-chlorophenyl)-3-hydroxy-1-methyl- 7-Chloro-5-(2-chlorophenyl)-3-hydroxy-1-methyl-2,3-dihydro-1H-1,4-benzodiazepin-2-one Methyllorazepam N-Methyllorazepam Ro 5-5516 7-Chloro-5-(o-chlorophenyl)-1,3-dihydro-3-hydroxy-1-methyl-2H-1,4-benzodiazepin-2-one Ergocalm Loramet Noctamid WY 4082 Noctamide
Inchi:	InChI=1S/C16H12Cl2N2O2/c1-20-13-7-6-9(17)8-11(13)14(19-15(21)16(20)22)10-4-2-3-5
InchiKey:	FJIKWRGCXUCUIG-UHFFFAOYSA-N
Formula:	C16H12Cl2N2O2
SMILES:	CN1C(=O)C(O)N=C(c2ccccc2Cl)c2cc(Cl)ccc21
Mol. weight [g/mol]:	335.19
CAS:	848-75-9

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.08		Crippen Method
logp	3.126		Crippen Method
mccvol	225.500	ml/mol	McGowan Method
rinpol	2674.00		NIST Webbook
rinpol	2703.00		NIST Webbook
rinpol	2674.00		NIST Webbook
rinpol	2798.40		NIST Webbook
rinpol	2717.00		NIST Webbook
rinpol	2703.00		NIST Webbook
rinpol	2703.00		NIST Webbook
rinpol	2753.00		NIST Webbook
rinpol	2674.00		NIST Webbook
rinpol	2717.00		NIST Webbook
rinpol	2674.00		NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C848759&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

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

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