

Clotiazepam

Other names:

2H-Thieno[2,3-e]-1,4-diazepin-2-one,
5-(2-chlorophenyl)-7-ethyl-1,3-dihydro-1-methyl-
2H-Thieno(2,3-e)(1,4)diazepin-2-one,
1,3-dihydro-5-(o-chlorophenyl)-7-ethyl-1-methyl-
5-(o-Chlorophenyl)-7-ethyl-1,3-dihydro-1-methyl-2H-thieno(2,3-e)-1,4-diazepin-2-one
5-(2-Chlorophenyl)-7-ethyl-1-methyl-1,3-dihydro-2H-thieno(2,3-e)(1,4)diazepin-2-one
Rize
2H-Thieno(2,3e)(1,4)-diazepin-2-one,
5-(o-chlorophenyl)-7-ethyl-1,3-dihydro-1-methyl-
Trecalmo
Y 6047
2H-Thieno[2,3-e]-1,4-diazepine-2-one,
5-(2-chlorophenyl)-7-ethyl-1,3-dihydro-1-methyl-
Clozan
Rize
Rizen
Tienor
Veratran
clothiazepam

Inchi: InChI=1S/C16H15ClN2OS/c1-3-10-8-12-15(11-6-4-5-7-13(11)17)18-9-14(20)19(2)16(12)
InchiKey: CHBRHODLKOZEPZ-UHFFFAOYSA-N
Formula: C16H15ClN2OS
SMILES: CCc1cc2c(s1)N(C)C(=O)CN=C2c1cccc1Cl
Mol. weight [g/mol]: 318.82
CAS: 33671-46-4

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.08		Crippen Method
logp	3.778		Crippen Method
mcvol	228.040	ml/mol	McGowan Method
rinpol	2513.00		NIST Webbook
rinpol	2485.00		NIST Webbook
rinpol	2513.00		NIST Webbook
rinpol	2540.00		NIST Webbook
rinpol	2530.00		NIST Webbook
rinpol	2540.00		NIST Webbook
rinpol	2485.00		NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C33671464&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307i
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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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