

Ketazolam

Other names:	4H-[1,3]Oxazino[3,2-d][1,4]benzodiazepine-4,7(6H)-dione, 11-chloro-8,12b-dihydro-2,8-dimethyl-12b-phenyl- Ansieten U 28774 U-28,774 Unakalm 11-Chloro-8,12b-dihydro-2,8-dimethyl-12b-phenyl-4H-(1,3)-oxazino(3,2-d)-(1,4)benzodiazepine-4,7(6H)-dione, 4H-(1,3)-Oxazino(3,2-d)-(1,4)benzodiazepine-4,7(6H)-dione, 11-chloro-8,12b-dihydro-2,8-dimethyl- 4H-(1,3)Oxazino(3,2-d)-(1,4)benzodiazepine-4,7(6H)-dione, 8,12b-dihydro-11-chloro-2,8-dimethyl-12b-phenyl- Anxon Anseren Contamex Loftran 11-Chloro-2,8-dimethyl-12b-phenyl-8,12b-dihydro-4H-[1,3]oxazino[3,2-d][1,4]benzodiazepine-4,7(6H)-dione, NSC 338158
Inchi:	InChI=1S/C20H17ClN2O3/c1-13-10-18(24)23-12-19(25)22(2)17-9-8-15(21)11-16(17)20(18,19)/h1-13,15-17,21-25
InchiKey:	PWAJCNITSBZRBL-UHFFFAOYSA-N
Formula:	C20H17ClN2O3
SMILES:	CC1=CC(=O)N2CC(=O)N(C)c3ccc(Cl)cc3C2(c2ccccc2)O1
Mol. weight [g/mol]:	368.81
CAS:	27223-35-4

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.27		Crippen Method
logp	3.280		Crippen Method
mcvol	260.330	ml/mol	McGowan Method
rinpol	2425.00		NIST Webbook
rinpol	2475.00		NIST Webbook
rinpol	2477.00		NIST Webbook
rinpol	2425.00		NIST Webbook

Sources

McGowan Method:

<http://link.springer.com/article/10.1007/BF02311772>

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C27223354&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
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
rinpolar: Non-polar retention indices

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