Clobazam

Other names:	1H-1,5-Benzodiazepine-2,4(3H,5H)-dione, 7-chloro-1-methyl-5-phenyl-
	Chlorepin
	Clorepin
	H 4723
	HR 376
	LM 2717
	RU-4723
	Urbanyl
	1-Phenyl-5-methyl-8-chloro-1,2,4,5-tetrahydro-2,4-dioxo-3H-1,5-benzodiazepine
	7-Chloro-1-methyl-5-phenyl-1H-1,5-benzodiazepine-2,4(3H,5H)-dione
	Frisium
	Urbadan
	Clobazepam
	NSC 336279
Inchi:	InChI=1S/C16H13ClN2O2/c1-18-13-8-7-11(17)9-14(13)19(16(21)10-15(18)20)12-5-3-2-4
InchiKey:	CXOXHMZGEKVPMT-UHFFFAOYSA-N
Formula:	C16H13ClN2O2
SMILES:	CN1C(=O)CC(=O)N(c2ccccc2)c2cc(Cl)ccc21
Mol. weight [g/mol]:	300.74
CAS:	22316-47-8

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.63		Crippen Method
logp	3.371		Crippen Method
mcvol	213.260	ml/mol	McGowan Method
rinpol	2582.00		NIST Webbook
rinpol	2582.00		NIST Webbook
rinpol	2565.00		NIST Webbook
rinpol	2647.60		NIST Webbook
rinpol	2605.00		NIST Webbook
rinpol	2582.00		NIST Webbook
rinpol	2582.00		NIST Webbook
rinpol	2559.00		NIST Webbook
rinpol	2557.00		NIST Webbook
tf	455.10 ± 0.50	K	NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C22316478&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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
rinpol:	Non-polar retention indices
tf:	Normal melting (fusion) point