Camazepam

Other names:	Carbamic acid, dimethyl-, 7-chloro-2,3-dihydro-1-methyl-2-oxo-5-phenyl-1H-1,4-benzodiazepin-3-yl ester Albego B 5333 7-Chloro-1,3-dihydro-3-(N,N-dimethylcarbamoyl)-1-methyl-5-phenyl-2H-1,4-benzodiazepi 7-Chloro-1,3-dihydro-3-hydroxy-1-methyl-5-phenyl-1,4-benzodiazepin-2-one dimethylcarbamate 3-N,N-Dimethylcarbamoyloxy-7-chloro-5-phenyl-1-methyl-1,3-dihydro-2H-1,4-benzodiaze SB 5833 7-Chloro-1,3-dihydro-3-hydroxy-1-methyl-5-phenyl-2H-1,4-benzodiazepin-2-one dimethylcarbamate (ester) Camazepam, (.+/-.)-
Inchi:	InChI=1S/C19H18ClN3O3/c1-22(2)19(25)26-17-18(24)23(3)15-10-9-13(20)11-14(15)16(2
InchiKey:	PXBVEXGRHZFEOF-UHFFFAOYSA-N
Formula:	C19H18ClN3O3
SMILES:	CN(C)C(=O)OC1N=C(c2ccccc2)c2cc(Cl)ccc2N(C)C1=O
Mol. weight [g/mol]:	371.82
CAS:	36104-80-0

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.79		Crippen Method
logp	3.178		Crippen Method
mcvol	267.080	ml/mol	McGowan Method
rinpol	2930.00		NIST Webbook
rinpol	2943.00		NIST Webbook
rinpol	2965.00		NIST Webbook
rinpol	2954.00		NIST Webbook
rinpol	2954.00		NIST Webbook
rinpol	2954.00		NIST Webbook
rinpol	2946.00		NIST Webbook
rinpol	2935.00		NIST Webbook
rinpol	2930.00		NIST Webbook
rinpol	2954.00		NIST Webbook

Sources

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=C36104800&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

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