Medazepam

Other names:	1H-1,4-Benzodiazepine, 2,3-dihydro-7-chloro-1-methyl-5-phenyl- 1H-1,4-Benzodiazepine, 7-chloro-2,3-dihydro-1-methyl-5-phenyl- 2,3-Dihydro-7-chloro-1-methyl-5-phenyl-1H-1,4-benzodiazepine 7-Chloro-2,3-dihydro-1-methyl-5-phenyl-1H-1,4-benzodiazepine 7-Chloro-2,3-dihydro-1-methyl-5-phenyl-3H-1,4-benzodiazepine 7-chloro-1-methyl-5-phenyl-2,3-dihydro-1,4-benzodiazepine Ansilan Enobrin Mezapam Narsis Nivelton Nobrium Psiquium Resmit Rudotel Tranquilax
Inchi:	InChI=1S/C16H15ClN2/c1-19-10-9-18-16(12-5-3-2-4-6-12)14-11-13(17)7-8-15(14)19/h2-
InchiKey:	YLCXGBZIZBEVPZ-UHFFFAOYSA-N
Formula:	C16H15ClN2
SMILES:	CN1CCN=C(c2ccccc2)c2cc(Cl)ccc21
Mol. weight [g/mol]:	270.76
CAS:	2898-12-6

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.75		Aqueous Solubility Prediction Method
logp	3.627		Crippen Method
mcvol	205.820	ml/mol	McGowan Method
rinpol	2272.00		NIST Webbook
rinpol	2275.00		NIST Webbook
rinpol	2243.00		NIST Webbook
rinpol	2285.00		NIST Webbook
rinpol	2235.00		NIST Webbook
rinpol	2226.00		NIST Webbook
rinpol	2287.00		NIST Webbook
rinpol	2287.00		NIST Webbook

rinpol	2270.00		NIST Webbook
rinpol	2240.00		NIST Webbook
rinpol	2226.00		NIST Webbook
rinpol	2285.00		NIST Webbook
rinpol	2235.00		NIST Webbook
rinpol	2226.00		NIST Webbook
rinpol	2272.00		NIST Webbook
rinpol	2287.00		NIST Webbook
tf	374.10 ± 0.50	K	NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C2898126&Units=SI

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Aqueous Solubility Prediction Method: http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa

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

rinpol: Non-polar retention indices

tf: Normal melting (fusion) point