Dimethazone

Other names:	2-[(2-chlorophenyl)methyl]-4,4-dimethyl-1,2-oxazolidin-3-one 2-[(2-chlorophenyl)methyl]-4,4-dimethyl-3-isoxazolidinone 3-Isoxazolidinone, 2-[(2-chlorophenyl)methyl]-4,4-dimethyl- Clomazone
Inchi:	InChI=1S/C12H14ClNO2/c1-12(2)8-16-14(11(12)15)7-9-5-3-4-6-10(9)13/h3-6H,7-8H2,1-
InchiKey:	KIEDNEWSYUYDSN-UHFFFAOYSA-N
Formula:	C12H14ClNO2
SMILES:	CC1(C)CON(Cc2ccccc2Cl)C1=O
Mol. weight [g/mol]:	239.70
CAS:	81777-89-1

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.34		Aqueous Solubility Prediction Method
log10ws	-2.34		Estimated Solubility Method
logp	2.640		Crippen Method
mcvol	174.980	ml/mol	McGowan Method
rinpol	1761.00		NIST Webbook
rinpol	1761.00		NIST Webbook

Sources

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
Estimated Solubility Method:	http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C81777891&Units=SI

Legend

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