

3H-1,4-Benzodiazepine, 2-amino-7-chloro-5-phenyl-, 4-oxide

Other names: 3H-1,4-Benzodiazepin-2-amine, 7-chloro-5-phenyl-, 4-oxide

Demethylclordiazepoxide

Desmethylclordiazepoxide

N-Demethylclordiazepoxide

N-Desmethylclordiazepoxide

Ro 5-0883

Inchi: InChI=1S/C15H12ClN3O/c16-11-6-7-13-12(8-11)15(10-4-2-1-3-5-10)19(20)9-14(17)18-1

InchiKey: LNLMGKOHYYEWMY-UHFFFAOYSA-N

Formula: C15H12ClN3O

SMILES: NC1=Nc2ccc(Cl)cc2C(c2ccccc2)=[N+][O-]C1

Mol. weight [g/mol]: 285.73

CAS: 7722-15-8

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.81		Crippen Method
logp	2.690		Crippen Method
mcpol	203.280	ml/mol	McGowan Method
rinpol	2885.00		NIST Webbook
rinpol	2885.00		NIST Webbook
rinpol	2885.00		NIST Webbook
rinpol	2930.00		NIST Webbook
rinpol	2885.00		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C7722158&Units=SI>

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

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

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