

Chlordiazepoxide

Other names: 3H-1,4-Benzodiazepin-2-amine, 7-chloro-N-methyl-5-phenyl-, 4-oxide
3H-1,4-Benzodiazepine, 2-methylamino-7-chloro-5-phenyl-4-oxide
3H-1,4-Benzodiazepine, 7-chloro-2-(methylamino)-5-phenyl-, 4-oxide
7-Chloro-2-methylamino-5-phenyl-3H-1,4-benzodiazepin-4-oxide
7-Chloro-2-methylamino-5-phenyl-3H-1,4-benzodiazepine 4-oxide
7-Cloro-2-metilamino-5-fenil-3H-1,4-benzodiazepina 4-ossido
7-chloro-N-methyl-5-phenyl-3H-1,4-benzodiazepin-2-amine 4-oxide
Abboxide
Balance
Balance (pharmaceutical)
Benzodiazepine-4-oxide, 7-chloro-2-methylamino-5-phenyl-3H-1,4-
CDO
Chloradiazepoxide
Chlordiazepoxid
Chloridazepoxide
Chloridiazepide
Chloridiazepoxide
Chlorodiazepoxide
Chlozepid
Clopoxide
Clordiazepossido
Control
Decacil
Eden
Elenium
Helogaphen
Ifibrium
Kalmocaps
Librelease
Librinin
Libritabs
Menrium
Mesural
Methaminodiazepoxide
Mildmen
Multum
Napoton
Napton
Psicosan
Radepur

Risolid
Silibrin
Tropium
Viopicol

Inchi: InChI=1S/C16H14ClN3O/c1-18-15-10-20(21)16(11-5-3-2-4-6-11)13-9-12(17)7-8-14(13)1
InchiKey: ANTSCNMPPGJYLG-UHFFFAOYSA-N
Formula: C16H14ClN3O
SMILES: CNC1=Nc2ccc(Cl)cc2C(c2ccccc2)=[N+][O-]C1
Mol. weight [g/mol]: 299.75
CAS: 58-25-3

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.39		Aqueous Solubility Prediction Method
logp	2.951		Crippen Method
mcpol	217.370	ml/mol	McGowan Method
rinpol	2778.00		NIST Webbook
rinpol	2774.00		NIST Webbook
rinpol	2809.00		NIST Webbook
rinpol	2825.00		NIST Webbook
rinpol	2780.00		NIST Webbook
rinpol	2926.40		NIST Webbook
rinpol	2798.00		NIST Webbook
rinpol	2764.00		NIST Webbook
rinpol	2778.00		NIST Webbook
rinpol	2815.00		NIST Webbook
rinpol	2774.00		NIST Webbook
rinpol	2799.00		NIST Webbook
rinpol	2815.00		NIST Webbook
rinpol	2815.00		NIST Webbook
rinpol	2808.00		NIST Webbook
rinpol	2820.00		NIST Webbook
rinpol	2820.00		NIST Webbook
rinpol	2742.00		NIST Webbook
rinpol	2799.00		NIST Webbook
rinpol	2742.00		NIST Webbook
rinpol	2780.00		NIST Webbook
tf	509.25	K	Aqueous Solubility Prediction Method

Sources

Crippen Method:

<http://pubs.acs.org/doi/abs/10.1021/ci990307l>

Solubility of Chlordiazepoxide,
Diazepam, and Lorazepam in Ethanol +
Water Mixtures at 303.2 K:

<https://www.doi.org/10.1021/je900200k>

Water Mixtures at 303.2 K:

<https://www.doi.org/10.1021/je900451d>

7-Chloro-2-methylamino-5-phenyl-3H-1,4-benzodiazepine-4-oxide,

7-Chloro-5-(2-methyl-5-phenyl-2H-1,4-benzodiazepin-2-ylidene)-

7-oxo-5,6-dihydro-2-methyl-5-phenyl-1,4-benzodiazepin-2-one,

and

7-Chloro-5-(2-chlorophenyl)-3-hydroxy-1,3-dihydro-1,4-benzodiazepin-2-one

<http://onlinelibrary.wiley.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDataset002.xlsx>

in (Propane-1,2-diol + Water) at a

Temperature of 303.2 K:

<http://link.springer.com/article/10.1007/BF02311772>

NIST Webbook

<http://webbook.nist.gov/cgi/cbook.cgi?ID=C58253&Units=SI>

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mccvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices
tf:	Normal melting (fusion) point

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