

Demoxepam

Other names:

2H-1,4-Benzodiazepin-2-one, 7-chloro-1,3-dihydro-5-phenyl-, 4-oxide
Chlordiazepoxide lactam
Ro 5-2092
Ro 5-2092 lactam
7-Chloro-1,3-dihydro-5-phenyl-2H-1,4-benzodiazepin-2-one 4-oxide
2H-1,4-Benzodiazepin-2-one, 1,3-dihydro-7-chloro-5-phenyl-, 4-oxide
1,3-Dihydro-7-chloro-5-phenyl-2H-1,4-benzodiazepin-2-one 4-oxide
NSC-46077
7-Chloro-1,3-dihydro-5-phenyl-2H-1,4-benzodiazepine-2-one N-oxide
NSC-46007
NSC 169898

Inchi:

InChI=1S/C15H11ClN2O2/c16-11-6-7-13-12(8-11)15(10-4-2-1-3-5-10)18(20)9-14(19)17-

InchiKey:

GGRWZBVSUZZMKS-UHFFFAOYSA-N

Formula:

C15H11ClN2O2

SMILES:

O=C1C[N+](O)=C(c2ccccc2)c2cc(Cl)ccc2N1

Mol. weight [g/mol]:

286.71

CAS:

963-39-3

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.51		Crippen Method
logp	2.640		Crippen Method
mcvol	199.170	ml/mol	McGowan Method

Sources

McGowan Method:

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

NIST Webbook:

<http://webbook.nist.gov/cgi/cbook.cgi?ID=C963393&Units=SI>

Crippen Method:

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

Crippen Method:

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

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume

Latest version available from:

<https://www.chemeo.com/cid/10-662-5/Demoxepam.pdf>

Generated by Cheméo on 2025-12-05 17:04:52.756792904 +0000 UTC m=+4702490.286833568.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.