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]:	286.72

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.74		Cheméo Relay (1.0)
logp	2.640		Crippen Method
mcvol	199.170	ml/mol	McGowan Method
tf	506.39	K	Cheméo Relay (1.0)

Sources

Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C963393&Units=SI
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
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
tf:	Normal melting (fusion) point