2H-1,4-Benzodiazepin-2-one, 7-chloro-1,3-dihydro-1-methyl-5-phenyl-3-[(trimetl

Other names: 7-Chloro-1-methyl-5-phenyl-3-[(trimethylsilyl)oxy]-1,3-dihydro-2H-1,4-benzodiazepin-2-on
Temazepam, TMS
Temazepam, trimethylsilyl ether

Inchi: InChI=1S/C19H21ClN2O2Si/c1-22-16-11-10-14(20)12-15(16)17(13-8-6-5-7-9-13)21-18(1

InchiKey: QQCHKHBRXNQGTF-UHFFFAOYSA-N

Formula: C19H21ClN2O2Si

SMILES: CN1C(=O)C(O[Si](C)(C)C)N=C(c2ccccc2)c2cc(Cl)ccc21

Mol. weight [g/mol]: 372.92

CAS: 35147-95-6

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.52		Crippen Method
logp	4.331		Crippen Method
rinpol	2646.90		NIST Webbook
rinpol	2646.90		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C35147956&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

rinpol: Non-polar retention indices