

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

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|-----------------------------|--|
| Other names: | 7-Chloro-1-methyl-5-phenyl-3-[(trimethylsilyloxy)]-1,3-dihydro-2H-1,4-benzodiazepin-2-one 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(19) |
| 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 |
| rinsol | 2646.90 | | NIST Webbook |
| rinsol | 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/ci9903071 |
| Crippen Method: | https://www.chemo.com/doc/models/crippen_log10ws |

Legend

| | |
|-----------------|-------------------------------------|
| log10ws: | Log10 of Water solubility in mol/l |
| logp: | Octanol/Water partition coefficient |
| rinsol: | Non-polar retention indices |

Latest version available from:

<https://www.chemo.com/cid/123-693-6/2H-1-4-Benzodiazepin-2-one-7-chloro-1-3-dihydro-1-methyl-5-phenyl-3-trime>

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