

«alpha»-Hydroxytriazolam, trimethylsilyl ether

Inchi: InChI=1S/C20H20Cl2N4OSi/c1-28(2,3)27-12-19-25-24-18-11-23-20(14-6-4-5-7-16(14)22
InchiKey: DEZQTJJZLGBSEX-UHFFFAOYSA-N
Formula: C20H20Cl2N4OSi
SMILES: C[Si](C)(C)OCc1nnc2n1-c1ccc(Cl)cc1C(c1cccc1Cl)=NC2
Mol. weight [g/mol]: 431.39

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.44		Crippen Method
logp	5.277		Crippen Method
rinpol	3203.40		NIST Webbook
rinpol	3203.40		NIST Webbook

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U417234&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

Legend

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

Latest version available from:

<https://www.chemeo.com/cid/80-452-1/alpha-Hydroxytriazolam-trimethylsilyl-ether.pdf>

Generated by Cheméo on 2024-04-25 13:55:49.097858998 +0000 UTC m=+16342598.018436313.

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