

«alpha»-Hydroxyalprazolam, trimethylsilyl ether

Inchi: InChI=1S/C20H21ClN4OSi/c1-27(2,3)26-13-19-24-23-18-12-22-20(14-7-5-4-6-8-14)16-1
InchiKey: NTTFKPLXWSKOKM-UHFFFAOYSA-N
Formula: C₂₀H₂₁ClN₄OSi
SMILES: C[Si](C)(C)OCc1nnc2n1-c1ccc(Cl)cc1C(c1ccccc1)=NC2
Mol. weight [g/mol]: 396.94

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.75		Crippen Method
logp	4.623		Crippen Method
rinpol	3087.70		NIST Webbook
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Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U417178&Units=SI>

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/80-455-8/alpha-Hydroxyalprazolam-trimethylsilyl-ether.pdf>

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