

Alprenolol, trimethylsilyl ether

Inchi: InChI=1S/C18H31NO2Si/c1-7-10-16-11-8-9-12-18(16)20-14-17(13-19-15(2)3)21-22(4,5)
InchiKey: IMNCYARVXPRPMP-UHFFFAOYSA-N
Formula: C18H31NO2Si
SMILES: C=CCc1ccccc1OCC(CNC(C)C)O[Si](C)(C)C
Mol. weight [g/mol]: 321.53

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.57		Crippen Method
logp	4.012		Crippen Method
rinpol	1864.60		NIST Webbook

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>
Crippen Method: https://www.cheméo.com/doc/models/crippen_log10ws
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U333830&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.cheméo.com/cid/59-285-1/Alprenolol-trimethylsilyl-ether.pdf>

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