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	-2.42		Cheméo Relay (1.0)
logp	4.012		Crippen Method
rinpol	1864.60		NIST Webbook
tf	306.79	K	Cheméo Relay (1.0)

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):
Cheméo Relay (1.0, beta):
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U333830&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
rinpol: Non-polar retention indices
tf: Normal melting (fusion) point

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