

cis-Tramadol, trimethylsilyl ether

Inchi: InChI=1S/C19H33NO2Si/c1-20(2)15-17-10-7-8-13-19(17,22-23(4,5)6)16-11-9-12-18(14-
InchiKey: KGLNMONDCPSZIK-UHFFFAOYSA-N
Formula: C19H33NO2Si
SMILES: COc1cccc(C2(O[Si](C)(C)C)CCCC2CN(C)C)c1
Mol. weight [g/mol]: 335.56

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.11		Crippen Method
logp	4.494		Crippen Method
rinpol	1975.80		NIST Webbook
rinpol	1975.80		NIST Webbook

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U417226&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/120-271-7/cis-Tramadol-trimethylsilyl-ether.pdf>

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