

N-Desmethyl-cis-tramadol, N-trimethylsilyl-, trimethylsilyl ether

Inchi: InChI=1S/C21H39NO2Si2/c1-22(25(3,4)5)17-19-12-9-10-15-21(19,24-26(6,7)8)18-13-11
InchiKey: WXEBJZUYUZCZOB-UHFFFAOYSA-N
Formula: C21H39NO2Si2
SMILES: COc1cccc(C2(O[Si](C)(C)C)CCCC2CN(C)[Si](C)(C)C)c1
Mol. weight [g/mol]: 393.71

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.00		Crippen Method
logp	5.699		Crippen Method
rinpol	2140.10		NIST Webbook
rinpol	2140.10		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U417187&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.cheméo.com/doc/models/crippen_log10ws

Legend

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

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