Norephedrine, N-isoBOC, O-TBDMS

Inchi: InChI=1S/C20H35NO3Si/c1-15(2)14-23-19(22)21-16(3)18(17-12-10-9-11-13-17)24-25(7,
InchiKey: KWCAVVIIBFBXAO-UHFFFAOYSA-N
Formula: C20H35NO3Si
SMILES: CC(C)COC(=O)NC(C)C(O[Si](C)(C)C(C)(C)C)c1ccccc1
Mol. weight [g/mol]: 365.58

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.79		Crippen Method
logp	5.520		Crippen Method
rinpol	2097.00		NIST Webbook
rinpol	2097.00		NIST Webbook

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=R392766&Units=SI

Legend

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

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