(1S2S)-Norephedrine, N-(2-phenylbutanoyl)-O-TMS

Inchi: InChI=1S/C22H31NO2Si/c1-6-20(18-13-9-7-10-14-18)22(24)23-17(2)21(25-26(3,4)5)19-1

InchiKey: NOHAOBDJBVQZRR-LYHOZKKVSA-N

Formula: C22H31NO2Si

SMILES: CCC(C(=O)NC(C)C(O[Si](C)(C)C)c1ccccc1)c1ccccc1

Mol. weight [g/mol]: 369.57

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.87		Crippen Method
logp	5.278		Crippen Method
rinpol	2240.00		NIST Webbook
rinpol	2240.00		NIST Webbook

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R99375&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

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