Norepinephrine, N-isoBOC, O-TBDMS

Inchi:	InChI=1S/C31H61NO5Si3/c1-23(2)22-34-28(33)32-21-27(37-40(16,17)31(9,10)11)24-18-
InchiKey:	HZPRZAZRYAOFIU-UHFFFAOYSA-N
Formula:	C31H61NO5Si3
SMILES:	CC(C)COC(=O)NCC(O[Si](C)(C)C(C)(C)C)c1ccc(O[Si](C)(C)C(C)(C)C)c(O[Si](C)(C)C(C
Mol. weight [g/mol]:	612.08

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.79		Crippen Method
logp	9.900		Crippen Method
rinpol	3205.00		NIST Webbook

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R392771&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

Latest version available from:

https://www.chemeo.com/cid/60-171-5/Norepinephrine-N-isoBOC-O-TBDMS.pdf

Generated by Cheméo on 2024-04-25 04:31:27.30788321 +0000 UTC m=+16308736.228460523.

Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.