DL-Norepinephrine, N,O,O',O''-tetrakis(trimethylsilyl)-

Other names: N-Pyrrol2-pyrrol3,4-bis[(trimethylsilyl)oxy]phenylmorpho-2-[(trimethylsilyl)oxy]ethylmorpho
Dl-norepinephrine, 4tms derivative

Inchi: InChI=1S/C20H43NO3Si4/c1-25(2,3)21-16-20(24-28(10,11)12)17-13-14-18(22-26(4,5)6)

InchiKey: MLHNBOALOLAGFS-UHFFFAOYSA-N

Formula: C20H43NO3Si4

SMILES: C[Si](C)(C)NCC(O[Si](C)(C)C)c1ccc(O[Si](C)(C)C)c(O[Si](C)(C)C)c1

Mol. weight [g/mol]: 457.90

Physical Properties

Property code	Value	Unit	Source
log10ws	2.36		Crippen Method
logp	6.431		Crippen Method
rinpol	1897.30		NIST Webbook
rinpol	1897.30		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U332935&Units=SI

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

rinpol: Non-polar retention indices