

9,12-Octadecadiynoic acid, trimethylsilyl ester

Inchi: InChI=1S/C21H36O2Si/c1-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-20-21(22)23-24(2,3)
InchiKey: PDBHHMKGVMRGBK-UHFFFAOYSA-N
Formula: C21H36O2Si
SMILES: CCCCC#CCC#CCCCCCCCC(=O)O[Si](C)(C)C
Mol. weight [g/mol]: 348.59

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.12		Crippen Method
logp	6.072		Crippen Method
rinpol	2311.20		NIST Webbook

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.cheméo.com/doc/models/crippen_log10ws
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U333566&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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