

Hexadecanoic acid, 2-[(trimethylsilyl)oxy]-, methyl ester

Other names: Hexadecanoic acid, 2-(trimethylsiloxy)-, methyl ester

Methylpalmitate, 2-trimethylsiloxy

Hexadecanoic acid, 2-hydroxy, methyl ester, TMS

Inchi: InChI=1S/C20H42O3Si/c1-6-7-8-9-10-11-12-13-14-15-16-17-18-19(20(21)22-2)23-24(3,4

InchiKey: ISYKTPYDGSSZAA-UHFFFAOYSA-N

Formula: C20H42O3Si

SMILES: CCCCCCCCCCCCCC(O[Si](C)(C)C)C(=O)OC

Mol. weight [g/mol]: 358.63

CAS: 21987-11-1

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.31		Crippen Method
logp	6.471		Crippen Method
rinpol	2124.00		NIST Webbook
rinpol	2126.00		NIST Webbook
rinpol	2124.00		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C21987111&Units=SI>

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

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

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