

Hexadecanoic acid, 16-(trimethylsiloxy)-, methyl ester

Other names: 16-hydroxyhexadecanoic acid, methyl ester TMSi ether
Inchi: InChI=1S/C20H42O3Si/c1-22-20(21)18-16-14-12-10-8-6-5-7-9-11-13-15-17-19-23-24(2,3)
InchiKey: XJKMNMXRQVIAK-UHFFFAOYSA-N
Formula: C20H42O3Si
SMILES: COC(=O)CCCCCCCCCCCCCCCCO[Si](C)(C)C
Mol. weight [g/mol]: 358.63
CAS: 21987-14-4

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|------|----------------|
| log10ws | -4.20 | | Crippen Method |
| logp | 6.472 | | Crippen Method |
| rinpol | 2268.00 | | NIST Webbook |
| rinpol | 2274.00 | | NIST Webbook |
| rinpol | 2268.00 | | NIST Webbook |
| rinpol | 2274.00 | | NIST Webbook |

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C21987144&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

Latest version available from:

<https://www.chemeo.com/cid/95-594-8/Hexadecanoic-acid-16-trimethylsiloxy-methyl-ester.pdf>

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