

Octanoic acid, 2-[(trimethylsilyl)oxy]-, trimethylsilyl ester-, (.+/-.)-

Other names:

Trimethylsilyl 2-[(trimethylsilyl)oxy]octanoate

Octanoic acid, 2-trimethylsilyloxy, trimethylsilyl ester

2-Hydroxyoctanoic acid, 2tms derivative

Inchi:

InChI=1S/C14H32O3Si2/c1-8-9-10-11-12-13(16-18(2,3)4)14(15)17-19(5,6)7/h13H,8-12H

InchiKey:

GMIHMOPIXUPKIA-UHFFFAOYSA-N

Formula:

C₁₄H₃₂O₃Si₂

SMILES:

CCCCCCC(O[Si](C)(C)C)C(=O)O[Si](C)(C)C

Mol. weight [g/mol]:

304.57

Physical Properties

Property code	Value	Unit	Source
log10ws	0.15		Crippen Method
logp	4.555		Crippen Method
rinpol	1440.00		NIST Webbook
rinpol	1464.00		NIST Webbook
rinpol	1464.00		NIST Webbook
rinpol	1440.00		NIST Webbook

Sources

NIST Webbook:

<http://webbook.nist.gov/cgi/cbook.cgi?ID=U332744&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.cheméo.com/cid/125-056-1/Octanoic-acid-2-trimethylsilyl-oxy-trimethylsilyl-ester.pdf>

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