

Octanoic acid, 2-[(tert-butyl dimethylsilyl)oxy]-, tert-butyl dimethylsilyl ester, (.+/-.)-

Other names: tert-Butyl(dimethyl)silyl 2-pyrrolidyl tert-butyl(dimethyl)silyloxymorpho-octanoate
Octanoic acid, 2-hydroxy, TBDMS

2-Hydroxyoctanoic acid, 2tdms derivative

Inchi: InChI=1S/C20H44O3Si2/c1-12-13-14-15-16-17(22-24(8,9)19(2,3)4)18(21)23-25(10,11)20

InchiKey: JGZSYPNWPQDUPE-UHFFFAOYSA-N

Formula: C20H44O3Si2

SMILES: CCCCCC(O[Si](C)(C)C(C)(C)C(=O)O[Si](C)(C)C(C)(C)C

Mol. weight [g/mol]: 388.73

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.36		Crippen Method
logp	6.896		Crippen Method
rinpol	1864.20		NIST Webbook
rinpol	1864.20		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=U332743&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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