

Hexacosanoic acid, tert-butyldimethylsilyl ester

Other names:	tert-Butyl(dimethyl)silyl hexacosanoate Hexacosanoic acid, TBDMS Cerotic acid, TBDMS Hexacosanoic acid, tbdms derivative
Inchi:	InChI=1S/C32H66O2Si/c1-7-8-9-10-11-12-13-14-15-16-17-18-19-20-21-22-23-24-25-26-
InchiKey:	OFXNWQJLALARIZ-UHFFFAOYSA-N
Formula:	C32H66O2Si
SMILES:	CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC(=O)O[Si](C)(C)C(C)(C)C
Mol. weight [g/mol]:	510.95

Physical Properties

Property code	Value	Unit	Source
log10ws	-10.13		Crippen Method
logp	11.917		Crippen Method
rinsol	3286.00		NIST Webbook
rinsol	3287.00		NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U333149&Units=SI

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
rinsol:	Non-polar retention indices

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<https://www.chemeo.com/cid/44-735-7/Hexacosanoic-acid-tert-butyldimethylsilyl-ester.pdf>

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