

Octadecanoic acid, tert-butyldimethylsilyl ester

Other names:	Octadecanoic acid, TBDMS Stearic acid, TBDMS Stearic acid, DMTBS tert-Butyl(dimethyl)silyl stearate Stearic acid, tbdms derivative
Inchi:	InChI=1S/C24H50O2Si/c1-7-8-9-10-11-12-13-14-15-16-17-18-19-20-21-22-23(25)26-27(
InchiKey:	KQJVB EYMSUXDQG-UHFFFAOYSA-N
Formula:	C24H50O2Si
SMILES:	CCCCCCCCCCCCCCCC(=O)O[Si](C)(C)C(C)(C)C
Mol. weight [g/mol]:	398.74
CAS:	87020-51-7

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.78		Crippen Method
logp	8.796		Crippen Method
rinpol	2489.00		NIST Webbook
rinpol	2486.70		NIST Webbook
rinpol	2490.00		NIST Webbook
rinpol	2476.00		NIST Webbook
rinpol	2486.70		NIST Webbook
rinpol	2489.00		NIST Webbook
rinpol	2482.80		NIST Webbook
rinpol	2489.00		NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C87020517&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/95-493-0/Octadecanoic-acid-tert-butyltrimethylsilyl-ester.pdf>

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