

Octadecanoic acid, trimethylsilyl ester

Other names:	Stearic acid, trimethylsilyl ester Trimethylsilyl ester of octadecanoic acid Trimethylsilyl stearate Octadecanoic acid, TMS Octadecanoic acid, TMS ester Stearoxytrimethylsilane Stearic acid, tms derivative
Inchi:	InChI=1S/C21H44O2Si/c1-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-20-21(22)23-24(2,3
InchiKey:	DDLDPZVTUKLKVQB-UHFFFAOYSA-N
Formula:	C21H44O2Si
SMILES:	CCCCCCCCCCCCCCCCC(=O)O[Si](C)(C)C
Mol. weight [g/mol]:	356.66
CAS:	18748-91-9

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.53		Crippen Method
logp	7.626		Crippen Method
rinpol	2243.00		NIST Webbook
rinpol	2236.43		NIST Webbook
rinpol	2207.00		NIST Webbook
rinpol	2240.00		NIST Webbook
rinpol	2238.00		NIST Webbook
rinpol	2242.00		NIST Webbook
rinpol	2243.00		NIST Webbook
rinpol	2238.00		NIST Webbook
rinpol	2239.00		NIST Webbook
rinpol	2234.10		NIST Webbook
rinpol	2239.00		NIST Webbook
rinpol	2239.00		NIST Webbook
rinpol	2248.00		NIST Webbook
rinpol	2250.00		NIST Webbook
rinpol	2252.00		NIST Webbook
rinpol	2239.00		NIST Webbook
rinpol	2255.00		NIST Webbook
rinpol	2250.00		NIST Webbook
rinpol	2244.00		NIST Webbook

rinpol	2243.00	NIST Webbook
rinpol	2247.00	NIST Webbook
rinpol	2255.00	NIST Webbook
rinpol	2247.00	NIST Webbook
rinpol	2244.00	NIST Webbook
rinpol	2248.00	NIST Webbook
rinpol	2242.00	NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C18748919&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

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