

Heptadecanoic acid, trimethylsilyl ester

Other names:	Heptadecanoic acid, TMS Heptadecanoic acid, TMS ester Margarate, TMS Margaric acid, trimethylsilyl ester Heptadecanoic acid, tms derivative
Inchi:	InChI=1S/C20H42O2Si/c1-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-20(21)22-23(2,3)4/
InchiKey:	KCEZRIREPDDPDI-UHFFFAOYSA-N
Formula:	C20H42O2Si
SMILES:	CCCCCCCCCCCCCCCC(=O)O[Si](C)(C)C
Mol. weight [g/mol]:	342.63
CAS:	55517-58-3

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.11		Crippen Method
logp	7.236		Crippen Method
rinpol	2152.00		NIST Webbook
rinpol	2144.00		NIST Webbook
rinpol	2137.40		NIST Webbook
rinpol	2148.00		NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C55517583&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/95-705-4/Heptadecanoic-acid-trimethylsilyl-ester.pdf>

Generated by Cheméo on 2024-04-20 05:16:17.075172932 +0000 UTC m=+15879425.995750254.

Cheméo (<https://www.cheméo.com>) is the biggest free database of chemical and physical data for the process industry.