Hexadecanoic acid, trimethylsilyl ester

Other names:	Palmitic acid, trimethylsilyl ester
	Hexadecanoic acid, TMS
	Hexadecanoic acid, TMS ester
	Palmitic acid, TMS
	Palmitic acid, tms derivative
Inchi:	InChI=1S/C19H40O2Si/c1-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19(20)21-22(2,3)4/h5-
InchiKey:	HKNNSWCACQFVIK-UHFFFAOYSA-N
Formula:	C19H40O2Si
SMILES:	CCCCCCCCCCCCCCCC(=O)O[Si](C)(C)C
Mol. weight [g/mol]:	328.61
CAS:	55520-89-3

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.69		Crippen Method
logp	6.846		Crippen Method
rinpol	2047.00		NIST Webbook
rinpol	2047.00		NIST Webbook
rinpol	2039.10		NIST Webbook
rinpol	2015.00		NIST Webbook
rinpol	2043.00		NIST Webbook
rinpol	2041.00		NIST Webbook
rinpol	2042.00		NIST Webbook
rinpol	2046.00		NIST Webbook
rinpol	2041.00		NIST Webbook
rinpol	2050.00		NIST Webbook
rinpol	2043.00		NIST Webbook
rinpol	2050.00		NIST Webbook
rinpol	2040.00		NIST Webbook
rinpol	2036.00		NIST Webbook
rinpol	2040.00		NIST Webbook
rinpol	2043.00		NIST Webbook
rinpol	2050.00		NIST Webbook
rinpol	2053.00		NIST Webbook
rinpol	2037.00		NIST Webbook
rinpol	2050.00		NIST Webbook
rinpol	2050.00		NIST Webbook

rinpol	2052.00	NIST Webbook
rinpol	2050.00	NIST Webbook
rinpol	2052.00	NIST Webbook
rinpol	2054.00	NIST Webbook
rinpol	2051.00	NIST Webbook
rinpol	2046.00	NIST Webbook
rinpol	2049.00	NIST Webbook
rinpol	2050.00	NIST Webbook
rinpol	2052.00	NIST Webbook
rinpol	2050.00	NIST Webbook
rinpol	2050.00	NIST Webbook
rinpol	2052.00	NIST Webbook
rinpol	2053.00	NIST Webbook
rinpol	2041.00	NIST Webbook
rinpol	2043.00	NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C55520893&Units=SI

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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