n-Tridecanoic acid, trimethylsilyl ester

Other names:	Tridecanoic acid, TMS
	Tridecanoic acid, trimethylsilyl ester
	Trimethylsilyl tridecanoate
	Tridecanoic acid, tms derivative
Inchi:	InChI=1S/C16H34O2Si/c1-5-6-7-8-9-10-11-12-13-14-15-16(17)18-19(2,3)4/h5-15H2,1-4H
InchiKey:	UZUTZCYXYDHJAT-UHFFFAOYSA-N
Formula:	C16H34O2Si
SMILES:	CCCCCCCCCCCCC(=O)O[Si](C)(C)C
Mol. weight [g/mol]:	286.53
CAS:	169597-14-2

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.43		Crippen Method
logp	5.676		Crippen Method
rinpol	1741.00		NIST Webbook
rinpol	1749.00		NIST Webbook
rinpol	1745.90		NIST Webbook
rinpol	1748.00		NIST Webbook
rinpol	1749.00		NIST Webbook
rinpol	1755.00		NIST Webbook
rinpol	1755.00		NIST Webbook
rinpol	1745.90		NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C169597142&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

Latest version available from:

https://www.chemeo.com/cid/65-366-4/n-Tridecanoic-acid-trimethylsilyl-ester.pdf

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