Undecanoic acid, tert-butyldimethylsilyl ester

Other names:	Undecanoic acid, TBDMS
	Undecanoic acid, DMTBS
	Undecanoic acid, tbdms derivative
Inchi:	InChI=1S/C17H36O2Si/c1-7-8-9-10-11-12-13-14-15-16(18)19-20(5,6)17(2,3)4/h7-15H2,1
InchiKey:	IJPQNIPLGFIDLM-UHFFFAOYSA-N
Formula:	C17H36O2Si
SMILES:	CCCCCCCCCCC(=O)O[Si](C)(C)C(C)(C)C
Mol. weight [g/mol]:	300.55
CAS:	104255-75-6

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.85		Crippen Method
logp	6.066		Crippen Method
rinpol	1781.60		NIST Webbook
rinpol	1782.00		NIST Webbook
rinpol	1784.00		NIST Webbook
rinpol	1773.00		NIST Webbook

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C104255756&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
rinpol:	Non-polar retention indices

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