Nonadecanoic acid, tert-butyldimethylsilyl ester

Other names:	Nonadecanoic acid, TBDMS
	tert-Butyl(dimethyl)silyl nonadecanoate
	Nonadecanoic acid, tbdms derivative
Inchi:	InChI=1S/C25H52O2Si/c1-7-8-9-10-11-12-13-14-15-16-17-18-19-20-21-22-23-24(26)27-
InchiKey:	IRJWTOHPSQRGKW-UHFFFAOYSA-N
Formula:	C25H52O2Si
SMILES:	CCCCCCCCCCCCCCCCCCC(=O)O[Si](C)(C)C(C)(C)C
Mol. weight [g/mol]:	412.76
CAS:	104255-82-5

Physical Properties

Property code	Value	Unit	Source
log10ws	-7.20		Crippen Method
logp	9.186		Crippen Method
rinpol	2583.80		NIST Webbook
rinpol	2589.00		NIST Webbook
rinpol	2576.00		NIST Webbook
rinpol	2583.80		NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C104255825&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/57-086-4/Nonadecanoic-acid-tert-butyldimethylsilyl-ester.pdf

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