

anteiso-Tridecanoic acid, TMS

Other names:	Dodecanoic acid, 10-methyl, trimethylsilyl ester
Inchi:	InChI=1S/C16H34O2Si/c1-6-15(2)13-11-9-7-8-10-12-14-16(17)18-19(3,4)5/h15H,6-14H2
InchiKey:	IHHDEEVODWBADL-UHFFFAOYSA-N
Formula:	C16H34O2Si
SMILES:	CCC(C)CCCCCCCC(=O)O[Si](C)(C)C
Mol. weight [g/mol]:	286.53

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.19		Crippen Method
logp	5.531		Crippen Method
rinpol	1717.00		NIST Webbook
rinpol	1717.00		NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R45390&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/38-811-9/anteiso-Tridecanoic-acid-TMS.pdf>

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