

11-Eicosenoic acid, DMTBS

Inchi:	InChI=1S/C26H52O2Si/c1-7-8-9-10-11-12-13-14-15-16-17-18-19-20-21-22-23-24-25(27)
InchiKey:	YYVUADHNPRFOCW-CCEZHUSRSA-N
Formula:	C26H52O2Si
SMILES:	CCCCCCCCC=CCCCCCCCCCC(=O)O[Si](C)(C)C(C)(C)C
Mol. weight [g/mol]:	424.78

Physical Properties

Property code	Value	Unit	Source
log10ws	-7.47		Crippen Method
logp	9.353		Crippen Method
rinpol	2621.00		NIST Webbook

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R537954&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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/52-348-8/11-Eicosenoic-acid-DMTBS.pdf>

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