cis-13-Docosenoic acid, tert-butyldimethylsilyl ester

Other names:	Erucic acid, TBDMS
	Erucic acid, DMTBS
	13-Docosenoic acid, (z)-, tbdms derivative
Inchi:	InChI=1S/C28H56O2Si/c1-7-8-9-10-11-12-13-14-15-16-17-18-19-20-21-22-23-24-25-26-
InchiKey:	ZFVWXEOSFGPVSH-PFONDFGASA-N
Formula:	C28H56O2Si
SMILES:	CCCCCCCCC=CCCCCCCCCCCCC(=O)O[Si](C)(C)C(C)(C)C
Mol. weight [g/mol]:	452.83

Physical Properties

Property code	Value	Unit	Source
log10ws	-8.31		Crippen Method
logp	10.133		Crippen Method
rinpol	2864.40		NIST Webbook
rinpol	2871.00		NIST Webbook
rinpol	2817.00		NIST Webbook
rinpol	2864.40		NIST Webbook

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U333241&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

Latest version available from:

https://www.chemeo.com/cid/31-020-4/cis-13-Docosenoic-acid-tert-butyldimethylsilyl-ester.pdf

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