

cis-4,7,10,13,16,19-Docosahexaenoic acid, tert-butyldimethylsilyl ester

Other names:	Doconexent, tbdms derivative
Inchi:	InChI=1S/C28H46O2Si/c1-7-8-9-10-11-12-13-14-15-16-17-18-19-20-21-22-23-24-25-26-
InchiKey:	CIORSZPTYHCMFP-MMRRFZAGSA-N
Formula:	C28H46O2Si
SMILES:	CCC=CCC=CCC=CCC=CCC=CCC=CCCC(=O)O[Si](C)(C)C(C)(C)C
Mol. weight [g/mol]:	442.75

Physical Properties

Property code	Value	Unit	Source
log10ws	-7.58		Crippen Method
logp	9.013		Crippen Method
rinsol	2811.90		NIST Webbook
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Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U333237&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

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

Latest version available from:

<https://www.chemeo.com/cid/69-118-5/cis-4-7-10-13-16-19-Docosahexaenoic-acid-tert-butyldimethylsilyl-ester.pdf>

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