

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

Other names:	Doconexent, tms derivative
Inchi:	InChI=1S/C25H40O2Si/c1-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-20-21-22-23-24-25
InchiKey:	WKGLYXNPWPPKPA-WSDBEMKQSA-N
Formula:	C25H40O2Si
SMILES:	CCC=CCC=CCC=CCC=CCC=CCC=CCCC(=O)O[Si](C)(C)C
Mol. weight [g/mol]:	400.67

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.32		Crippen Method
logp	7.842		Crippen Method
rinpol	2562.20		NIST Webbook

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U333238&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

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<https://www.chemeo.com/cid/12-455-3/cis-4-7-10-13-16-19-Docosahexaenoic-acid-trimethylsilyl-ester.pdf>

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