

cis-5,8,11,14,17-Eicosapentaenoic acid, tert-butyldimethylsilyl ester

Other names:	Eicosapentaenoic acid, tbdms derivative
Inchi:	InChI=1S/C26H44O2Si/c1-7-8-9-10-11-12-13-14-15-16-17-18-19-20-21-22-23-24-25(27)
InchiKey:	HOCHZABOEHUCRO-QXPWYRSVSA-N
Formula:	C26H44O2Si
SMILES:	CCC=CCC=CCC=CCC=CCC=CCCCC(=O)O[Si](C)(C)C(C)(C)C
Mol. weight [g/mol]:	416.71

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.89		Crippen Method
logp	8.457		Crippen Method
rinsol	2627.10		NIST Webbook
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Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U333531&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

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<https://www.chemeo.com/cid/86-500-1/cis-5-8-11-14-17-Eicosapentaenoic-acid-tert-butyldimethylsilyl-ester.pdf>

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