

Hexacosanoic acid, trimethylsilyl ester

Other names:	Hexacosanoic acid, TMS Hexacosanoic acid, tms derivative
Inchi:	InChI=1S/C29H60O2Si/c1-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-20-21-22-23-24-25
InchiKey:	BHIAWJAQCOESNE-UHFFFAOYSA-N
Formula:	C ₂₉ H ₆₀ O ₂ Si
SMILES:	<chem>CCCCCCCCCCCCCCCCCCCCCCCCCC(=O)O[Si](C)(C)C</chem>
Mol. weight [g/mol]:	468.87

Physical Properties

Property code	Value	Unit	Source
log10ws	-8.88		Crippen Method
logp	10.747		Crippen Method
rinpol	3006.70		NIST Webbook
rinpol	3045.00		NIST Webbook
rinpol	3033.00		NIST Webbook
rinpol	3045.00		NIST Webbook
rinpol	3033.00		NIST Webbook

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U333861&Units=SI>

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/48-571-5/Hexacosanoic-acid-trimethylsilyl-ester.pdf>

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