

Eicosanoic acid, trimethylsilyl ester

Other names:	Arachidic acid, trimethylsilyl ester Eicosanoic acid, TMS ester Eicosanoic acid, TMS Arachidic acid, tms derivative
Inchi:	InChI=1S/C23H48O2Si/c1-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-20-21-22-23(24)25
InchiKey:	AYSGFBVOWSXJCN-UHFFFAOYSA-N
Formula:	C23H48O2Si
SMILES:	CCCCCCCCCCCCCCCCCCCC(=O)O[Si](C)(C)C
Mol. weight [g/mol]:	384.71
CAS:	55530-70-6

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.36		Crippen Method
logp	8.406		Crippen Method
rinpol	2416.85		NIST Webbook
rinpol	2437.00		NIST Webbook
rinpol	2454.00		NIST Webbook
rinpol	2447.00		NIST Webbook
rinpol	2451.00		NIST Webbook
rinpol	2442.00		NIST Webbook
rinpol	2451.00		NIST Webbook
rinpol	2456.00		NIST Webbook
rinpol	2454.00		NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C55530706&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
rinpol: Non-polar retention indices

Latest version available from:

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