

trans-9-Octadecenoic acid, trimethylsilyl ester

Other names:	Trimethylsilyl (9E)-9-octadecenoate TMS trans-9-octadecenoate (E)-9-Octadecenoic acid, TMS ester trans-9-Octadecenoic acid, TMS 9-Octadecenoic acid, (e)-, tms derivative
Inchi:	InChI=1S/C21H42O2Si/c1-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-20-21(22)23-24(2,3)
InchiKey:	GAODWSYPSJBKGB-OUKQBFOZSA-N
Formula:	C21H42O2Si
SMILES:	CCCCCCCCC=CCCCCCCC(=O)O[Si](C)(C)C
Mol. weight [g/mol]:	354.64
CAS:	96851-47-7

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.38		Crippen Method
logp	7.402		Crippen Method
rinpol	2215.05		NIST Webbook
rinpol	2217.70		NIST Webbook
rinpol	2227.00		NIST Webbook
rinpol	2227.00		NIST Webbook
rinpol	2215.05		NIST Webbook
rinpol	2217.70		NIST Webbook

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C96851477&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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