

trans-Traumatic acid, bis(trimethylsilyl) ester

Other names:	Traumatic acid, (e)-, 2tms derivative
Inchi:	InChI=1S/C18H36O4Si2/c1-23(2,3)21-17(19)15-13-11-9-7-8-10-12-14-16-18(20)22-24(4
InchiKey:	XUSCELGAZUEVPT-FYWRMAATSA-N
Formula:	C18H36O4Si2
SMILES:	C[Si](C)(C)OC(=O)C=CCCCCCCCC(=O)O[Si](C)(C)C
Mol. weight [g/mol]:	372.65

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.04		Crippen Method
logp	5.420		Crippen Method
rinpol	2135.40		NIST Webbook
rinpol	2123.00		NIST Webbook
rinpol	2131.00		NIST Webbook
rinpol	2135.40		NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U352405&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws

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.cheméo.com/cid/124-687-2/trans-Traumatic-acid-bis-trimethylsilyl-ester.pdf>

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