

Tocopherol-«gamma»-tms-derivative (high mass adjustment=100%)

Other names:	Tocopherol-«gamma»-tms-derivative (high mass adjustment=50%) Tocopherol-«gamma»-tms-derivative (high mass adjustment=0%) (+)-.gamma.-Tocopherol, O-trimethylsilyl-
Inchi:	InChI=1S/C31H56O2Si/c1-23(2)14-11-15-24(3)16-12-17-25(4)18-13-20-31(7)21-19-28-2
InchiKey:	PQZJQAFFNUIVLK-UHFFFAOYSA-N
Formula:	C31H56O2Si
SMILES:	<chem>Cc1c(O[Si](C)(C)C)cc2c(c1C)OC(C)(CCCC(C)CCCC(C)CCCC(C)C)CC2</chem>
Mol. weight [g/mol]:	488.86
CAS:	2733-27-9

Physical Properties

Property code	Value	Unit	Source
log10ws	-8.75		Crippen Method
logp	10.040		Crippen Method
rinpol	3014.00		NIST Webbook
rinpol	2999.00		NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C2733279&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/46-840-8/Tocopherol-gamma-tms-derivative-high-mass-adjustment-100.pdf>

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