

Simvastatin, trimethylsilyl ether

Other names:	Simvastatin, tms derivative
Inchi:	InChI=1S/C28H46O5Si/c1-9-28(4,5)27(30)32-24-15-18(2)14-20-11-10-19(3)23(26(20)24
InchiKey:	SUEDSISDIUMYSI-UHFFFAOYSA-N
Formula:	C28H46O5Si
SMILES:	CCC(C)(C)C(=O)OC1CC(C)C=C2C=CC(C)C(CCC3CC(O[Si](C)(C)C)CC(=O)O3)C21
Mol. weight [g/mol]:	490.75

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.93		Crippen Method
logp	6.445		Crippen Method
rinpol	3142.00		NIST Webbook
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Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U334006&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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:

<https://www.chemeo.com/cid/87-827-8/Simvastatin-trimethylsilyl-ether.pdf>

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