

Warfarin, O-trimethylsilyl-

Other names:	Warfarin, trimethylsilyl ether Warfarin, TMS Warfarin, tms derivative
Inchi:	InChI=1S/C22H24O4Si/c1-15(23)14-18(16-10-6-5-7-11-16)20-21(26-27(2,3)4)17-12-8-9-
InchiKey:	ZGTLYCBMQNUUBB-UHFFFAOYSA-N
Formula:	C22H24O4Si
SMILES:	CC(=O)CC(c1cccc1)c1c(O[Si](C)(C)C)c2cccc2oc1=O
Mol. weight [g/mol]:	380.51
CAS:	36307-79-6

Physical Properties

Property code	Value	Unit	Source
log10ws	-8.04		Crippen Method
logp	5.118		Crippen Method
rinpol	2718.40		NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C36307796&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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/77-641-5/Warfarin-O-trimethylsilyl.pdf>

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