Warfarin, tert-butyldimethylsilyl ether

Other names: Warfarin, tbdms derivative
Inchi: InChI=1S/C25H30O4Si/c1-17(26)16-20(18-12-8-7-9-13-18)22-23(29-30(5,6)25(2,3)4)19-
InchiKey: LVUJUTVWWDLBSD-UHFFFAOYSA-N
Formula: C25H30O4Si
SMILES: CC(=O)CC(c1ccccc1)c1c(O[Si](C)(C)C(C)(C)C)c2ccccc2oc1=O
Mol. weight [g/mol]: 422.60

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.06		Cheméo Relay (1.0)
logp	6.288		Crippen Method
rinpol	2935.50		NIST Webbook
tf	400.96	K	Cheméo Relay (1.0)

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):
Cheméo Relay (1.0, beta):
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U333974&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
rinpol: Non-polar retention indices
tf: Normal melting (fusion) point

Latest version available from:
https://www.chemeo.com/cid/12-403-0/Warfarin-tert-butyldimethylsilyl-ether.pdf

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