

28-Norcastasterone, methaneboronate-TMS ether

Inchi:	InChI=1S/C34H63BO5Si2/c1-21(2)17-30(39-41(7,8)9)32(40-42(10,11)12)22(3)24-13-14-
InchiKey:	IOXYGWCXWZRYJG-UADYOINTSA-N
Formula:	C34H63BO5Si2
SMILES:	CB1OC2CC3C(=O)CC4C(CCC5(C)C(C(C)C(O[Si](C)(C)C)C(CC(C)C)O[Si](C)(C)C)CCC
Mol. weight [g/mol]:	618.84

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.20		Crippen Method
logp	8.459		Crippen Method
rinpol	3533.00		NIST Webbook
rinpol	3533.00		NIST Webbook
rinpol	3533.00		NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R499951&Units=SI

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/16-356-9/28-Norcastasterone-methaneboronate-TMS-ether.pdf>

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