

6-Deoxocasterone, methaneboronate-TMS ether

Inchi:	InChI=1S/C35H67BO4Si2/c1-22(2)23(3)32(39-41(8,9)10)33(40-42(11,12)13)24(4)27-16-
InchiKey:	QKLDQTPNZPFYAV-YOYWPEALSA-N
Formula:	C35H67BO4Si2
SMILES:	CB1OC2CC3CCC4C(CCC5(C)C(C(C)C(O[Si](C)(C)C)C(O[Si](C)(C)C)C(C)C(C)C)CCC4
Mol. weight [g/mol]:	618.89

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.10		Crippen Method
logp	9.526		Crippen Method
rinpol	3428.00		NIST Webbook
rinpol	3429.00		NIST Webbook
rinpol	3428.00		NIST Webbook

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R499966&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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/61-755-6/6-Deoxocasterone-methaneboronate-TMS-ether.pdf>

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