

Bolasterone, TMS

Other names:	Bolasterone, 17-TMS
Inchi:	InChI=1S/C24H40O2Si/c1-16-14-17-15-18(25)8-11-22(17,2)19-9-12-23(3)20(21(16)19)1
InchiKey:	YODBBXQVBBUISJ-OLLNBOXPXA-N
Formula:	C ₂₄ H ₄₀ O ₂ Si
SMILES:	CC1CC2=CC(=O)CCC2(C)C2CCC3(C)C(CCC3(C)O[Si](C)(C)C)C12
Mol. weight [g/mol]:	388.66

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.38		Crippen Method
logp	6.375		Crippen Method
rinsol	2828.00		NIST Webbook
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Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R55042&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
rinsol:	Non-polar retention indices

Latest version available from:

<https://www.chemeo.com/cid/51-585-6/Bolasterone-TMS.pdf>

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