

5«alpha»-Androstane-3,17-dione, 2-enol, per-TMS

Inchi:	InChI=1S/C25H44O2Si2/c1-24-15-13-19(26-28(3,4)5)17-18(24)9-10-20-21-11-12-23(27-
InchiKey:	RJIVKCCIVQDMHQ-OOTJLFDSSA-N
Formula:	C25H44O2Si2
SMILES:	CC12CCC3C(CCC4CC(O[Si](C)(C)C)=CCC43C)C1CC=C2O[Si](C)(C)C
Mol. weight [g/mol]:	432.79

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.39		Crippen Method
logp	7.720		Crippen Method
rinpol	2669.00		NIST Webbook

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R518542&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/39-901-8/5-alpha-Androstane-3-17-dione-2-enol-per-TMS.pdf>

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