

1,3(5«beta»)-androsten-3,17«beta»-diol di-TMS

Other names:	5«beta»-Androst-1-en-17«beta»-ol-3-one, 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:	MHYUVCDDDLAFJG-VTHHSRKNSA-N
Formula:	C25H44O2Si2
SMILES:	CC12C=CC(O[Si](C)(C)C)=CC1CCC1C2CCC2(C)C(O[Si](C)(C)C)CCC12
Mol. weight [g/mol]:	432.79

Physical Properties

Property code	Value	Unit	Source
logp	7.370		Crippen Method
rinpol	2467.00		NIST Webbook
rinpol	2467.00		NIST Webbook
rinpol	2480.00		NIST Webbook
rinpol	2474.00		NIST Webbook
rinpol	2493.00		NIST Webbook
rinpol	2474.00		NIST Webbook

Sources

Cheméo Relay (1.0, beta):

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R172928&Units=SI>

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Cheméo Relay (1.0):

Legend

logp: Octanol/Water partition coefficient

rinpol: Non-polar retention indices

Latest version available from:

<https://www.cheméo.com/cid/122-427-2/1-3-5-beta-androsten-3-17-beta-diol-di-TMS.pdf>

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