

5«alpha»-Androstan-3,17-dione, 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: BMWSYFZMLBIPOC-OOTJLFDSSA-N
Formula: C25H44O2Si2
SMILES: CC12CCC3C(CCC4C=C(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
logp	7.720		Crippen Method
rinpol	2645.00		NIST Webbook
rinpol	2660.00		NIST Webbook
rinpol	2645.00		NIST Webbook
rinpol	2649.00		NIST Webbook
rinpol	2660.00		NIST Webbook

Sources

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R321789&Units=SI>

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

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

Legend

logp: Octanol/Water partition coefficient

rinpol: Non-polar retention indices

Latest version available from:

<https://www.chemeo.com/cid/125-049-9/5-alpha-Androstan-3-17-dione-TMS.pdf>

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