

4-Androsten-3-«alpha»,17-«alpha»-diol, TMS

Inchi: InChI=1S/C25H46O2Si2/c1-24-15-13-19(26-28(3,4)5)17-18(24)9-10-20-21-11-12-23(27-28)/h1-10,12-14,16,18,20-22,24-25,27-28H,23H2,26H3
InchiKey: APMJYCGLEHJTKS-AGDHPOHRSA-N
Formula: C25H46O2Si2
SMILES: CC12CCC(O[Si](C)(C)C)C=C1CCC1C2CCC2(C)C(O[Si](C)(C)C)CCC12
Mol. weight [g/mol]: 434.80

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.32		Cheméo Relay (1.0)
logp	7.389		Crippen Method
rinpol	2444.00		NIST Webbook
rinpol	2444.00		NIST Webbook
rinpol	2426.00		NIST Webbook
rinpol	2475.00		NIST Webbook
rinpol	2426.00		NIST Webbook
tf	365.77	K	Cheméo Relay (1.0)

Sources

Cheméo Relay (1.0, beta):

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R384557&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

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
rinpol: Non-polar retention indices
tf: Normal melting (fusion) point

Latest version available from:

<https://www.chemeo.com/cid/119-021-6/4-Androsten-3-alpha-17-alpha-diol-TMS.pdf>

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