

Clostebol M (Androst-4-en-4-chloro-3A-ol-17-one), TMS

Inchi: InChI=1S/C25H43ClO2Si2/c1-24-16-14-21(27-29(3,4)5)23(26)20(24)10-9-17-18-11-12-2
InchiKey: SHTZVTGOIGPHTA-UHFFFAOYSA-N
Formula: C₂₅H₄₃ClO₂Si₂
SMILES: CC12CCC3C(CCC4=C(Cl)C(O[Si](C)(C)C)CCC43C)C1CC=C2O[Si](C)(C)C
Mol. weight [g/mol]: 467.23

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.90		Crippen Method
logp	8.081		Crippen Method
rinpol	2720.00		NIST Webbook
rinpol	2720.00		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U412248&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.cheméo.com/doc/models/crippen_log10ws

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.cheméo.com/cid/116-401-7/Clostebol-M-Androst-4-en-4-chloro-3A-ol-17-one-TMS.pdf>

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