

5«alpha»-Androstane-3,6,17-trione, TMS

Inchi: InChI=1S/C25H42O3Si2/c1-24-13-11-17(27-29(3,4)5)15-21(24)22(26)16-18-19-9-10-23(24)
InchiKey: QWPVJBAFROZYRV-AZCQQNBGSA-N
Formula: C₂₅H₄₂O₃Si₂
SMILES: CC12CCC3C(CC(=O)C4CC(O[Si](C)(C)C)=CCC43C)C1CC=C2O[Si](C)(C)C
Mol. weight [g/mol]: 446.77

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.67		Crippen Method
logp	6.899		Crippen Method
rinpol	2789.00		NIST Webbook
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Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R307065&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>

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/61-544-0/5-alpha-Androstane-3-6-17-trione-TMS.pdf>

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