

5«alpha»-Androstane-3,7,17-trione, TMS

Inchi: InChI=1S/C25H42O3Si2/c1-24-13-11-18(27-29(3,4)5)15-17(24)16-21(26)23-19-9-10-22(23)
InchiKey: MQUYMUUVPOKMNN-DZSZRFSFSA-N
Formula: C₂₅H₄₂O₃Si₂
SMILES: CC12CCC3C(C(=O)CC4CC(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	2584.00		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=R307070&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/25-994-1/5-alpha-Androstane-3-7-17-trione-TMS.pdf>

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