

5«alpha»-Androstan-17«beta»-ol-3-one, VDMS

Inchi: InChI=1S/C23H38O2Si/c1-6-26(4,5)25-21-10-9-19-18-8-7-16-15-17(24)11-13-22(16,2)20
InchiKey: BQMPHVFWKDRPIA-RNAHECHESA-N
Formula: C23H38O2Si
SMILES: C=C[Si](C)(C)OC1CCC2C3CCC4CC(=O)CCC4(C)C3CCC12C
Mol. weight [g/mol]: 374.63

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.05		Crippen Method
logp	5.914		Crippen Method
rinpol	2658.00		NIST Webbook
rinpol	2658.00		NIST Webbook

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R529314&Units=SI>

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/11-862-2/5-alpha-Androstan-17-beta-ol-3-one-VDMS.pdf>

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