

Dehydroepiandrosterone, TBDMSi (3-O)

Inchi: InChI=1S/C25H42O2Si/c1-23(2,3)28(6,7)27-18-12-14-24(4)17(16-18)8-9-19-20-10-11-22
InchiKey: BGIQEPPPFPSKLP-CSUWYVEXSA-N
Formula: C25H42O2Si
SMILES: CC12CCC3C(CC=C4CC(O[Si](C)(C)C(C)(C)C)CCC43C)C1CCC2=O
Mol. weight [g/mol]: 402.69

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.04		Crippen Method
logp	6.909		Crippen Method
rinpol	2803.00		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R144582&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>
Crippen Method: https://www.chemeo.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.chemeo.com/cid/63-362-0/Dehydroepiandrosterone-TBDMSi-3-O.pdf>

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