

Androst-5-en-11-one, 3,17-bis[(trimethylsilyl)oxy]-, (3«beta»,17«beta»)-

Other names:

3,17-Bis[(trimethylsilyl)oxy]androst-5-en-11-one, (3«beta»,17«beta»)-
3B,17B-Dihydroxy-5-androstene, bis-TMS

Inchi: InChI=1S/C25H44O3Si2/c1-24-14-13-18(27-29(3,4)5)15-17(24)9-10-19-20-11-12-22(28-30)-31
InchiKey: MBBKELNLMOIAQM-VHVWKQIRSA-N
Formula: C25H44O3Si2
SMILES: CC12CCC(O[Si](C)(C)C)CC1=CCC1C2C(=O)CC2(C)C(O[Si](C)(C)C)CCC12
Mol. weight [g/mol]: 448.79
CAS: 49774-90-5

Physical Properties

Property code	Value	Unit	Source
logp	6.568		Crippen Method
rinpol	2620.00		NIST Webbook
rinpol	2620.00		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C49774905&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>
Crippen Method: https://www.cheméo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):
Cheméo Relay (1.0, beta):

Legend

logp: Octanol/Water partition coefficient
rinpol: Non-polar retention indices

Latest version available from:
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