

trans-Dehydroandrosterone, trimethylsilyl ether

Other names:

(3«beta»)-3-[(Trimethylsilyl)oxy]androst-5-en-17-one

Dehydroepiandrosterone, (e)-, tms derivative

Inchi:

InChI=1S/C22H36O2Si/c1-21-12-10-16(24-25(3,4)5)14-15(21)6-7-17-18-8-9-20(23)22(18)

InchiKey:

BVHPVDOXVFBYNL-UHFFFAOYSA-N

Formula:

C₂₂H₃₆O₂Si

SMILES:

CC12CCC3C(CC=C4CC(O[Si](C)(C)C)CCC43C)C1CCC2=O

Mol. weight [g/mol]:

360.61

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.79		Crippen Method
logp	5.738		Crippen Method
rinpol	2623.30		NIST Webbook

Sources

NIST Webbook:

<http://webbook.nist.gov/cgi/cbook.cgi?ID=U332999&Units=SI>

Crippen Method:

<http://pubs.acs.org/doi/abs/10.1021/ci9903071>

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/13-828-8/trans-Dehydroandrosterone-trimethylsilyl-ether.pdf>

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