

5«alpha»-Androst-16-en-3«beta»-ol trimethylsilyl ether

Other names: 3-[(Trimethylsilyl)oxy]androst-16-ene, (5«alpha»,3«beta»)-5«alpha»-Androst-16-en-3«beta»-ol, TMS
5-«alpha»,16-Androsten-3-«beta»-ol, TMS
Androst-16-en-3-ol, (3«beta»,5«alpha»)-, tms derivative

Inchi: InChI=1S/C22H38OSi/c1-21-12-6-7-19(21)18-9-8-16-15-17(23-24(3,4)5)10-14-22(16,2)2

InchiKey: HUNGYZOAGOETMS-UHFFFAOYSA-N

Formula: C22H38OSi

SMILES: CC12C=CCC1C1CCC3CC(O[Si](C)(C)C)CCC3(C)C1CC2

Mol. weight [g/mol]: 346.62

CAS: 56210-81-2

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|------|----------------|
| log10ws | -4.26 | | Crippen Method |
| logp | 6.415 | | Crippen Method |
| rinpol | 2245.00 | | NIST Webbook |

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C56210812&Units=SI>

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

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/36-842-7/5-alpha-Androst-16-en-3-beta-ol-trimethylsilyl-ether.pdf>

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