

Pregn-5-en-20-one, 3-[(trimethylsilyl)oxy]-, (3«beta»)-

Other names:

Pregn-5-en-20-one, 3«beta»-(trimethylsiloxy)-
Pregnenolone trimethylsilyl ether
3«beta»-Trimethylsilyloxypregn-5-en-20-one
Trimethylsilyl derivative of 3«beta»-hydroxypregn-5-en-20-one
3-[(Trimethylsilyl)oxy]pregn-5-en-20-one, (3«beta»)-
5-Pregnen-3«beta»-ol-20-one, trimethylsilyl ether
3-[(Trimethylsilyl)oxy]pregn-5-en-20-one
Pregnenolone, tms derivative

Inchi: InChI=1S/C24H40O2Si/c1-16(25)20-9-10-21-19-8-7-17-15-18(26-27(4,5)6)11-13-23(17,2

InchiKey: MQAKMQDJWRHTAA-UHFFFAOYSA-N

Formula: C24H40O2Si

SMILES: CC(=O)C1CCC2C3CC=C4CC(O[Si](C)(C)C)CCC4(C)C3CCC12C

Mol. weight [g/mol]: 388.66

CAS: 18919-58-9

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.38		Crippen Method
logp	6.375		Crippen Method
rinpol	2784.30		NIST Webbook
rinpol	2695.00		NIST Webbook
rinpol	2695.00		NIST Webbook

Sources

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

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C18919589&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

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