

Pregn-5-en-20-one, 3«beta»-(trimethylsiloxy)-, O-methyloxime

Other names:	Pregnenolone, MO-TMS
Inchi:	InChI=1S/C25H43NO2Si/c1-17(26-27-4)21-10-11-22-20-9-8-18-16-19(28-29(5,6)7)12-14
InchiKey:	UJRFOJLCOGKWOK-ZBZGGUAESA-N
Formula:	C25H43NO2Si
SMILES:	CON=C(C)C1CCC2C3CC=C4CC(O[Si](C)(C)C)CCC4(C)C3CCC12C
Mol. weight [g/mol]:	417.70
CAS:	25830-38-0

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.76		Crippen Method
logp	6.808		Crippen Method
rinpola	2834.00		NIST Webbook
rinpola	2834.00		NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C25830380&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
rinpola:	Non-polar retention indices

Latest version available from:

<https://www.chemeo.com/cid/71-643-9/Pregn-5-en-20-one-3-beta-trimethylsiloxy-O-methyloxime.pdf>

Generated by Cheméo on 2024-04-27 04:00:24.796898803 +0000 UTC m=+16479673.717476118.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.