

21-Hydroxyprogesterone, trimethylsilyl ether, bis(O-methyloxime)

Other names:	21-Hydroxy-4-pregnen-3,20-dione, MO TMS
Inchi:	InChI=1S/C26H44N2O3Si/c1-25-14-12-19(27-29-3)16-18(25)8-9-20-21-10-11-23(26(21,2
InchiKey:	QDEFZWVWFGZSRJ-UHFFFAOYSA-N
Formula:	C26H44N2O3Si
SMILES:	CON=C1C=C2CCC3C(CCC4(C)C(C(CO[Si](C)(C)C)=NOC)CCC34)C2(C)CC1
Mol. weight [g/mol]:	460.72

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.31		Crippen Method
logp	6.422		Crippen Method
rinpol	3066.00		NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U394487&Units=SI

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/71-373-9/21-Hydroxyprogesterone-trimethylsilyl-ether-bis-O-methyloxime.pdf>

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