

5-«alpha»-Pregnan-3-«beta»-ol-20-one, TMS

Other names:	5-«alpha»-Pregnan-3-«beta»-ol-20-one, MeTMS
Inchi:	InChI=1S/C24H42O2Si/c1-16(25)20-9-10-21-19-8-7-17-15-18(26-27(4,5)6)11-13-23(17,2
InchiKey:	GKHMQSZBQGVKC-MIWXRYBXSA-N
Formula:	C24H42O2Si
SMILES:	CC(=O)C1CCC2C3CCC4CC(O[Si](C)(C)C)CCC4(C)C3CCC12C
Mol. weight [g/mol]:	390.67

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.29		Crippen Method
logp	6.454		Crippen Method
rinsol	2705.00		NIST Webbook
rinsol	2705.00		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=R393427&Units=SI

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
rinsol:	Non-polar retention indices

Latest version available from:

<https://www.chemeo.com/cid/20-150-2/5-alpha-Pregnan-3-beta-ol-20-one-TMS.pdf>

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