

3.alpha.-hydroxy-pregn-4-en-20-one, MO-TMS

Other names:	3«alpha»-Dihydroprogesterone, 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:	JVLYJNBVYMT OHS-OAJKAGJUSA-N
Formula:	C25H43NO2Si
SMILES:	CO/N=C(\C)[C@H]1CCC2C3CCC4=C[C@H](O[Si](C)(C)C)CC[C@]4(C)C3CC[C@@]21
Mol. weight [g/mol]:	417.71

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.63		Cheméo Relay (1.0)
logp	6.808		Crippen Method
tf	401.24	K	Cheméo Relay (1.0)

Sources

Cheméo Relay (1.0, beta):

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?Str2File=R395785>

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>

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

Cheméo Relay (1.0):

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
tf:	Normal melting (fusion) point

Latest version available from:

<https://www.chemeo.com/cid/115-936-5/3-alpha-hydroxy-pregn-4-en-20-one-MO-TMS.pdf>

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