

20«alpha»-hydroxy-pregn-4-en-3-one, MO-TMS, syn

Inchi: InChI=1S/C25H43NO2Si/c1-17(28-29(5,6)7)21-10-11-22-20-9-8-18-16-19(26-27-4)12-14
InchiKey: ROBQPFGUYCNUGC-UWCRPIHPSA-N
Formula: C25H43NO2Si
SMILES: CON=C1C=C2CCC3C(CCC4(C)C(C(C)O[Si](C)(C)C)CCC34)C2(C)CC1
Mol. weight [g/mol]: 417.70

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.46		Cheméo Relay (1.0)
logp	6.808		Crippen Method
rinpol	2933.00		NIST Webbook
rinpol	2933.00		NIST Webbook
tf	389.70	K	Cheméo Relay (1.0)

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R395765&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307I>
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):
Cheméo Relay (1.0, beta):

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
rinpol: Non-polar retention indices
tf: Normal melting (fusion) point

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