

5-Pregnen-3-«beta»-20-one, TMS

Inchi: InChI=1S/C24H40O2Si/c1-16(25)20-9-10-21-19-8-7-17-15-18(26-27(4,5)6)11-13-23(17,24)
InchiKey: MQAKMQDJWRHTAA-XVSKKSDESA-N
Formula: C₂₄H₄₀O₂Si
SMILES: CC(=O)C1CCC2C3CC=C4CC(O[Si](C)(C)C)CCC4(C)C3CCC12C
Mol. weight [g/mol]: 388.66

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.38		Crippen Method
logp	6.375		Crippen Method
rinpol	2694.00		NIST Webbook

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>
Crippen Method: https://www.cheméo.com/doc/models/crippen_log10ws
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R499604&Units=SI>

Legend

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

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