

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

Inchi: InChI=1S/C25H45NO2Si/c1-17(28-29(5,6)7)21-10-11-22-20-9-8-18-16-19(26-27-4)12-14
InchiKey: MEPCJQMOKOWTNN-QPGYPTNSSA-N
Formula: C25H45NO2Si
SMILES: CON=C1CCC2(C)C(CCC3C2CCC2(C)C(C(C)O[Si](C)(C)C)CCC32)C1
Mol. weight [g/mol]: 419.72

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.67		Crippen Method
logp	6.888		Crippen Method
rinpol	2757.00		NIST Webbook

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.cheméo.com/doc/models/crippen_log10ws
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R486881&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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