

Pregnan-2,3-diol-20-one, MeTMS

Inchi: InChI=1S/C27H50O3Si2/c1-18(28)21-12-13-22-20-11-10-19-16-24(29-31(4,5)6)25(30-32)
InchiKey: MBKAWRRRLZQGDS-AHAXGFRTSA-N
Formula: C27H50O3Si2
SMILES: CC(=O)C1CCC2C3CCC4CC(O[Si](C)(C)C)C(O[Si](C)(C)C)CC4(C)C3CCC12C
Mol. weight [g/mol]: 478.86

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.79		Crippen Method
logp	7.284		Crippen Method
rinpol	2804.00		NIST Webbook
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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=R393645&Units=SI>

Legend

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

Latest version available from:

<https://www.chemeo.com/cid/31-420-0/Pregnan-2-3-diol-20-one-MeTMS.pdf>

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