

5.beta.-Pregnane-20-one-3.alpha.,21-diol, TMSO-TMS, # 1

Inchi: InChI=1S/C29H57NO3Si3/c1-29-18-17-24-23-14-12-22(32-35(5,6)7)19-21(23)11-13-25(26,27)28
InchiKey: QXSFCLWTCIYKPY-ZQDHXNOASA-N
Formula: C29H57NO3Si3
SMILES: C[C@]12CCC3C(CC[C@@H]4C[C@H](O[Si](C)(C)C)CCC34)C1CC[C@@H]2C(CO[Si](C)(C)C)C5[Si](C)(C)C5
Mol. weight [g/mol]: 552.04

Physical Properties

Property code	Value	Unit	Source
logp	8.534		Crippen Method

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R527105&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>
Crippen Method: https://www.cheméo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):
Cheméo Relay (1.0, beta):

Legend

logp: Octanol/Water partition coefficient

Latest version available from:

<https://www.cheméo.com/cid/70-010-2/5-beta-Pregnane-20-one-3-alpha-21-diol-TMSO-TMS-1.pdf>

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