

5.beta.-Pregnane-20-one-3.alpha.,21-diol, EO-TMS, # 2

Inchi: InChI=1S/C28H53NO3Si2/c1-9-30-29-27(19-31-33(3,4)5)26-15-14-25-24-12-10-20-18-21
InchiKey: KJZKGCMYIBJAAZ-APPFXLQNSA-N
Formula: C28H53NO3Si2
SMILES: CCON=C(CO[Si](C)(C)C)[C@H]1CCC2C3CC[C@@H]4C[C@H](O[Si](C)(C)C)CCC4C3
Mol. weight [g/mol]: 507.91

Physical Properties

Property code	Value	Unit	Source
logp	7.719		Crippen Method

Sources

Cheméo Relay (1.0, beta):

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?Str2File=R527076>

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Cheméo Relay (1.0):

Legend

logp: Octanol/Water partition coefficient

Latest version available from:

<https://www.chemeo.com/cid/121-093-4/5-beta-Pregnane-20-one-3-alpha-21-diol-EO-TMS-2.pdf>

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