

«beta»-Cortolone, tris-TMS

Inchi: InChI=1S/C30H58O5Si3/c1-28-16-14-22(34-37(6,7)8)18-21(28)12-13-23-24-15-17-30(32)
InchiKey: RPGCPBZHIXGQ-HVZZIZDUSA-N
Formula: C30H58O5Si3
SMILES: CC12CCC(O[Si](C)(C)C)CC1CCC1C2C(=O)CC2(C)C1CCC2(O)C(CO[Si](C)(C)C)O[Si](C)(C)C
Mol. weight [g/mol]: 583.03

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.80		Crippen Method
logp	7.231		Crippen Method
rinpol	3092.00		NIST Webbook
rinpol	3092.00		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R16527&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.cheméo.com/doc/models/crippen_log10ws

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.cheméo.com/cid/67-408-5/beta-Cortolone-tris-TMS.pdf>

Generated by Cheméo on 2024-04-27 04:07:17.219101135 +0000 UTC m=+16480086.139678452.

Cheméo (<https://www.cheméo.com>) is the biggest free database of chemical and physical data for the process industry.