

«alpha»-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-YGGMGLDSA-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	3060.00		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R16509&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/55-548-3/alpha-Cortolone-tris-TMS.pdf>

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