

Cortolone MO TMS

Inchi: InChI=1S/C34H69NO5Si4/c1-32-20-18-26(38-42(7,8)9)22-25(32)16-17-27-28-19-21-34(4)
InchiKey: XELWYCNVFGIFEQ-KAMNWEAPSA-N
Formula: C34H69NO5Si4
SMILES: CON=C1CC2(C)C(CCC2(O[Si](C)(C)C)C(CO[Si](C)(C)C)O[Si](C)(C)C)C2CCC3CC(O[Si](C)(C)C)C3
Mol. weight [g/mol]: 684.26

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|------|----------------|
| log10ws | -0.31 | | Crippen Method |
| logp | 9.523 | | Crippen Method |
| rinpol | 3068.00 | | NIST Webbook |
| rinpol | 3050.00 | | NIST Webbook |
| rinpol | 3048.00 | | NIST Webbook |
| rinpol | 3071.00 | | NIST Webbook |
| rinpol | 3071.00 | | NIST Webbook |
| rinpol | 3068.00 | | NIST Webbook |
| rinpol | 3067.00 | | NIST Webbook |
| rinpol | 3065.00 | | NIST Webbook |

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R92737&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

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/29-868-7/Cortolone-MO-TMS.pdf>

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