

24-Methylenecholesterol, TMS

Inchi: InChI=1S/C31H56OSi/c1-21(2)10-11-22(3)23(4)27-14-15-28-26-13-12-24-20-25(32-33(7)
InchiKey: YFOZZKUJEPCKKZ-MDHOEFNSSA-N
Formula: C31H56OSi
SMILES: C=C(CCC(C)C)C(C)C1CCC2C3CCC4CC(O[Si](C)(C)C)CCC4(C)C3CCC12C
Mol. weight [g/mol]: 472.86

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|------|----------------|
| log10ws | -7.31 | | Crippen Method |
| logp | 9.494 | | Crippen Method |
| rinpol | 3230.00 | | NIST Webbook |

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R528693&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/64-687-9/24-Methylenecholesterol-TMS.pdf>

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