

Brassicasterol, TMS

Inchi: InChI=1S/C31H54OSi/c1-21(2)22(3)10-11-23(4)27-14-15-28-26-13-12-24-20-25(32-33(7)
InchiKey: OUZPLOOSCBQQGW-ITLMFHBGSA-N
Formula: C31H54OSi
SMILES: CC(C)C(C)C=CC(C)C1CCC2C3CC=C4CC(O[Si](C)(C)C)CCC4(C)C3CCC12C
Mol. weight [g/mol]: 470.85

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|------|----------------|
| log10ws | -7.16 | | Crippen Method |
| logp | 9.270 | | Crippen Method |
| rinpol | 3185.00 | | NIST Webbook |
| rinpol | 3185.00 | | NIST Webbook |

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R528940&Units=SI>

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.chemeo.com/cid/46-979-5/Brassicasterol-TMS.pdf>

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