

Cannabidiol, allyl-DMS

Inchi: InChI=1S/C31H50O2Si2/c1-11-14-15-16-26-22-29(32-34(7,8)19-12-2)31(30(23-26)33-35)
InchiKey: LQVLXLSBZAMCKD-QXPUDEPPSA-N
Formula: C31H50O2Si2
SMILES: C=CC[Si](C)(C)Oc1cc(CCCCC)cc(O[Si](C)(C)CC=C)c1C1C=C(C)CCC1C(=C)C
Mol. weight [g/mol]: 510.90

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|------|----------------|
| log10ws | -6.40 | | Crippen Method |
| logp | 9.975 | | Crippen Method |
| rinpol | 2565.00 | | NIST Webbook |
| rinpol | 2565.00 | | NIST Webbook |

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R526355&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>

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/48-488-8/Cannabidiol-allyl-DMS.pdf>

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