

cannabidiolic acid, TMS

Inchi: InChI=1S/C31H54O4Si3/c1-14-15-16-17-24-21-27(33-36(5,6)7)29(26-20-23(4)18-19-25(30,31)22)32
InchiKey: NLUDHDUQAJYEEH-FTJBHMTQSA-N
Formula: C31H54O4Si3
SMILES: C=C(C)C1CCC(C)=CC1c1c(O[Si](C)(C)C)cc(CCCCC)c(C(=O)O[Si](C)(C)C)c1O[Si](C)(C)C
Mol. weight [g/mol]: 575.01

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.15		Crippen Method
logp	9.854		Crippen Method
rinpol	2532.00		NIST Webbook
rinpol	2532.00		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=R487557&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/98-961-7/cannabidiolic-acid-TMS.pdf>

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