

1(7)-Tetrahydrocannabinol, TBDMS

Inchi: InChI=1S/C27H44O2Si/c1-10-11-12-13-20-17-23-25(24(18-20)29-30(8,9)26(3,4)5)21-16
InchiKey: SVRFTGVMSZGQLA-FOIFJWKZSA-N
Formula: C27H44O2Si
SMILES: C=C1CCC2C(C1)c1c(cc(CCCCC)cc1O[Si](C)(C)C(C)(C)C)OC2(C)C
Mol. weight [g/mol]: 428.72

Physical Properties

Property code	Value	Unit	Source
log10ws	-7.12		Crippen Method
logp	8.414		Crippen Method
rinpol	2559.00		NIST Webbook
rinpol	2559.00		NIST Webbook

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R525921&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/46-871-4/1-7-Tetrahydrocannabinol-TBDMS.pdf>

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