

Propyl-1-tetrahydrocannabinol, TMS

Inchi: InChI=1S/C22H34O2Si/c1-8-9-16-13-19-21(20(14-16)24-25(5,6)7)17-12-15(2)10-11-18(1)
InchiKey: UFMMSWJZLXGVQG-QRWMCTBCSA-N
Formula: C22H34O2Si
SMILES: CCCc1cc2c(c(O[Si](C)(C)C)c1)C1C=C(C)CCC1C(C)(C)O2
Mol. weight [g/mol]: 358.59

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.03		Crippen Method
logp	6.464		Crippen Method
rinpol	2170.00		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=R526464&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/40-426-4/Propyl-1-tetrahydrocannabinol-TMS.pdf>

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