

Cannabinol, TMS

Inchi: InChI=1S/C24H38O2Si/c1-8-9-10-11-18-15-21-23(22(16-18)26-27(5,6)7)19-14-17(2)12-1
InchiKey: JFPSLJJGWCHYOE-ANYOKISRSA-N
Formula: C24H38O2Si
SMILES: CCCCCc1cc2c(c(O[Si](C)(C)C)c1)C1C=C(C)CCC1C(C)(C)O2
Mol. weight [g/mol]: 386.64

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.87		Crippen Method
logp	7.244		Crippen Method
rinpol	2430.00		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=R526404&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/41-911-4/Cannabinol-TMS.pdf>

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