

Nabilone, tert-butyldimethylsilyl ether

Other names:	Nabilone, tbdms derivative
Inchi:	InChI=1S/C30H50O3Si/c1-11-12-13-14-17-29(5,6)21-18-25-27(26(19-21)33-34(9,10)28(
InchiKey:	YZWOEKHKXFJRKW-UHFFFAOYSA-N
Formula:	C30H50O3Si
SMILES:	CCCCCCC(C)(C)c1cc2c(c(O[Si](C)(C)C(C)(C)C)c1)C1CC(=O)CCC1C(C)(C)O2
Mol. weight [g/mol]:	486.80

Physical Properties

Property code	Value	Unit	Source
log10ws	-7.48		Crippen Method
logp	8.942		Crippen Method
rinpol	2933.40		NIST Webbook

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U352969&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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/12-098-0/Nabilone-tert-butyldimethylsilyl-ether.pdf>

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