

Nabilone, trimethylsilyl ether

Other names:	Nabilone, tms derivative
Inchi:	InChI=1S/C27H44O3Si/c1-9-10-11-12-15-26(2,3)19-16-23-25(24(17-19)30-31(6,7)8)21-1
InchiKey:	HGNFBYPDELVTBF-UHFFFAOYSA-N
Formula:	C27H44O3Si
SMILES:	CCCCCCC(C)(C)c1cc2c(c(O[Si](C)(C)C)c1)C1CC(=O)CCC1C(C)(C)O2
Mol. weight [g/mol]:	444.72

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.22		Crippen Method
logp	7.772		Crippen Method
rinpol	2724.40		NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U352970&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/37-454-7/Nabilone-trimethylsilyl-ether.pdf>

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