

MELATONIN 2TMS

Other names:	Melatonin, TMS
Inchi:	InChI=1S/C19H32N2O2Si2/c1-15(23-25(6,7)8)20-12-11-16-14-21(24(3,4)5)19-10-9-17(2
InchiKey:	LLIYBEZPSWVSDX-UHFFFAOYSA-N
Formula:	C19H32N2O2Si2
SMILES:	COc1ccc2c(c1)c(CCN=C(C)O[Si](C)(C)C)cn2[Si](C)(C)C
Mol. weight [g/mol]:	376.64

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.43		Crippen Method
logp	5.145		Crippen Method
rinpol	2378.00		NIST Webbook
rinpol	2364.00		NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R95096&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/48-650-7/MELATONIN-2TMS.pdf>

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