

Sterigmatocystin, O-tert.-butyldimethylsilyl-

Inchi:	InChI=1S/C24H26O6Si/c1-24(2,3)31(5,6)30-15-9-7-8-14-19(15)21(25)20-16(26-4)12-17-
InchiKey:	HERDFAHEKSFMAK-UHFFFAOYSA-N
Formula:	C24H26O6Si
SMILES:	COc1cc2c(c3oc4cccc(O[Si](C)(C)C(C)(C)C)c4c(=O)c13)C1C=COC1O2
Mol. weight [g/mol]:	438.55

Physical Properties

Property code	Value	Unit	Source
log10ws	-9.76		Crippen Method
logp	5.685		Crippen Method
rinpol	3302.00		NIST Webbook
rinpol	3302.00		NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U374667&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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/72-400-7/Sterigmatocystin-O-tert-butyldimethylsilyl.pdf>

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