

cis-Catechin, pentakis-TMS

Other names:	cis-Catechin, penta-TMS
Inchi:	InChI=1S/C30H54O6Si5/c1-37(2,3)32-23-19-26-24(27(20-23)34-39(7,8)9)21-29(36-41(1
InchiKey:	QKMSLFRFGOTVEJ-LOYHVIPDSA-N
Formula:	C30H54O6Si5
SMILES:	C[Si](C)(C)Oc1cc2c(c(O[Si](C)(C)C)c1)CC(O[Si](C)(C)C)C(c1ccc(O[Si](C)(C)C)c(O[Si](C
Mol. weight [g/mol]:	651.17

Physical Properties

Property code	Value	Unit	Source
log10ws	1.10		Crippen Method
logp	9.438		Crippen Method
rinpola	2912.00		NIST Webbook
rinpola	2913.00		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=R573425&Units=SI

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
rinpola:	Non-polar retention indices

Latest version available from:

<https://www.chemeo.com/cid/44-746-5/cis-Catechin-pentakis-TMS.pdf>

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