

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(13,14)15)30-31
InchiKey: QKMSLFRFGOTVEJ-IHLOFXLRSA-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)(C)C)c1)C
Mol. weight [g/mol]: 651.17

Physical Properties

Property code	Value	Unit	Source
log10ws	1.10		Crippen Method
logp	9.438		Crippen Method
rinpol	2934.00		NIST Webbook

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>
Crippen Method: https://www.cheméo.com/doc/models/crippen_log10ws
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R570179&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.cheméo.com/cid/70-620-5/Catechin-penta-TMS.pdf>

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