2H-1-Benzopyran, 3,4-dihydro-2-[3,4-bis[(trimethylsilyl)oxy]phenyl]-3,5,7-tris[(trimethylsilyl)oxy]-, (2R-trans)-

Other names: 1(2H)-Benzopyran, 3,4-dihydro-2-[3,4-bis[(trimethylsilyl)oxy]phenyl]-3,5,7-tris[(trimethylsilyl)oxy]-, (2R-trans)-
Catechin, penta-TMS ether
Catechin, TMS
Catechine (2r-e)-, 5tms derivative

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

InchiKey: QKMSLFRFGOTVEJ-UHFFFAOYSA-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

CAS: 64138-54-1

Physical Properties

Property code	Value	Unit	Source
log10ws	1.10		Crippen Method
logp	9.438		Crippen Method
rinpol	2860.40		NIST Webbook
rinpol	2938.00		NIST Webbook
rinpol	2943.00		NIST Webbook
rinpol	2938.00		NIST Webbook
rinpol	2898.80		NIST Webbook

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C64138541&Units=SI

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

rinpol: Non-polar retention indices