

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)-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(12,13)14)30-25-22-18-17-16-15-11-10-8-7-6-5-4-3-2
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)(C)C)c1)C2
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

rinpola: Non-polar retention indices

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