

Silane, [[2-[3,4-bis[(trimethylsilyl)oxy]phenyl]-3,4-dihydro-2H-1-benzopyran-3-yl]oxy]-2-methylpropane-1-thiol, (2R-cis)-

Other names:

Catechine, penta-TMS-ether, (2R-cis)-

Epicatechine, penta-TMS-ether

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(10,11)12)30-38

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)(C)C)c1)C

Mol. weight [g/mol]: 651.17

CAS: 89267-68-5

Physical Properties

Property code	Value	Unit	Source
log10ws	1.10		Crippen Method
logp	9.438		Crippen Method
rinpol	2838.20		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C89267685&Units=SI>

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

Crippen Method: https://www.cheméo.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.cheméo.com/cid/71-822-0/Silane-2-3-4-bis-trimethylsilyl-oxy-phenyl-3-4-dihydro-2H-1-benzopyran-3-5-7-yl-2-methylpropane-1-thiol-\(2R-cis\)-](https://www.cheméo.com/cid/71-822-0/Silane-2-3-4-bis-trimethylsilyl-oxy-phenyl-3-4-dihydro-2H-1-benzopyran-3-5-7-yl-2-methylpropane-1-thiol-(2R-cis)-)

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