

(4-Hydroxy-3-methoxyphenyl)ethylene glycol tris(trimethylsilyl) ether

Other names:

4-Hydroxy-3-methoxyphenylene glycol triTMS
1,2-Ethanediol, 4-hydroxy-3-methoxyphenyl, tris-TMS
4-Hydroxy-3-methoxyphenylglycol, 3tms derivative

Inchi: InChI=1S/C18H36O4Si3/c1-19-17-13-15(11-12-16(17)21-24(5,6)7)18(22-25(8,9)10)14-20

InchiKey: AAFYLSSHQRPLSR-UHFFFAOYSA-N

Formula: C18H36O4Si3

SMILES: COc1cc(C(CO[Si](C)(C)C)O[Si](C)(C)C)ccc1O[Si](C)(C)C

Mol. weight [g/mol]: 400.73

CAS: 68595-81-3

Physical Properties

Property code	Value	Unit	Source
log10ws	1.35		Crippen Method
logp	5.653		Crippen Method
rinpol	1850.00		NIST Webbook

Sources

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

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C68595813&Units=SI>

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

Legend

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

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<https://www.chemeo.com/cid/59-579-5/4-Hydroxy-3-methoxyphenyl-ethylene-glycol-tris-trimethylsilyl-ether.pdf>

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