

# Tocopherol-«delta»-tms-derivative (high mass adjustment=100%)

Other names:

Tocopherol-«delta»-tms-derivative (high mass adjustment=0%)

Tocopherol-«delta»-tms-derivative (high mass adjustment=50%)

.delta.-Tocopherol, O-trimethylsilyl-

Inchi:

InChI=1S/C30H54O2Si/c1-23(2)13-10-14-24(3)15-11-16-25(4)17-12-19-30(6)20-18-27-2

InchiKey:

OCAXNUPKBRKNKO-UHFFFAOYSA-N

Formula:

C30H54O2Si

SMILES:

Cc1cc(O[Si](C)(C)C)cc2c1OC(C)(CCCC(C)CCCC(C)CCCC(C)C)CC2

Mol. weight [g/mol]:

474.83

CAS:

52704-11-7

## Physical Properties

| Property code | Value   | Unit | Source         |
|---------------|---------|------|----------------|
| log10ws       | -8.28   |      | Crippen Method |
| logp          | 9.732   |      | Crippen Method |
| rinpol        | 2900.00 |      | NIST Webbook   |
| rinpol        | 2913.00 |      | NIST Webbook   |

## Sources

Crippen Method:

[https://www.chemeo.com/doc/models/crippen\\_log10ws](https://www.chemeo.com/doc/models/crippen_log10ws)

NIST Webbook:

<http://webbook.nist.gov/cgi/cbook.cgi?ID=C52704117&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

Latest version available from:

<https://www.chemeo.com/cid/98-921-1/Tocopherol-delta-tms-derivative-high-mass-adjustment-100.pdf>

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