

Pentaerythritol, TMS

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|-----------------------------|--|
| Other names: | 2,2,8,8-tetramethyl-5,5-bis[[trimethylsilyloxy]methyl]-3,7-dioxa-2,8-disilanonane |
| Inchi: | InChI=1S/C17H44O4Si4/c1-22(2,3)18-13-17(14-19-23(4,5)6,15-20-24(7,8)9)16-21-25(10) |
| InchiKey: | DCRQMOJXJXVZFC-UHFFFAOYSA-N |
| Formula: | C17H44O4Si4 |
| SMILES: | C[Si](C)(C)OCC(CO[Si](C)(C)C)(CO[Si](C)(C)C)CO[Si](C)(C)C |
| Mol. weight [g/mol]: | 424.87 |
| CAS: | 2114-25-2 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|------|----------------|
| log10ws | 4.75 | | Crippen Method |
| logp | 5.379 | | Crippen Method |
| rinpol | 1535.00 | | NIST Webbook |

Sources

| | |
|------------------------|---|
| Crippen Method: | http://pubs.acs.org/doi/abs/10.1021/ci9903071 |
| Crippen Method: | https://www.chemeo.com/doc/models/crippen_log10ws |
| NIST Webbook: | http://webbook.nist.gov/cgi/cbook.cgi?ID=C2114252&Units=SI |

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/41-753-0/Pentaerythritol-TMS.pdf>

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