

trans-4-Octenedioic acid, TMS

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|-----------------------------|---|
| Inchi: | InChI=1S/C14H28O4Si2/c1-19(2,3)17-13(15)11-9-7-8-10-12-14(16)18-20(4,5)6/h7-8H,9- |
| InchiKey: | ZMVKLEZAWZSWHA-BQYQJAHWSA-N |
| Formula: | C14H28O4Si2 |
| SMILES: | C[Si](C)(C)OC(=O)CCC=CCCC(=O)O[Si](C)(C)C |
| Mol. weight [g/mol]: | 316.54 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|------|----------------|
| log10ws | 0.64 | | Crippen Method |
| logp | 3.859 | | Crippen Method |
| rinpol | 1684.00 | | NIST Webbook |

Sources

| | |
|------------------------|---|
| NIST Webbook: | http://webbook.nist.gov/cgi/cbook.cgi?ID=R584004&Units=SI |
| Crippen Method: | http://pubs.acs.org/doi/abs/10.1021/ci9903071 |
| 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 |

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