

Butanoic acid, 4-[(trimethylsilyl)oxy]-, trimethylsilyl ester

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|-----------------------------|---|
| Other names: | Butyric acid, 4-(trimethylsiloxy)-, trimethylsilyl ester «gamma»-Hydroxybutyric acid (2TMS) 4-Hydroxybutyric acid, (2TMS)- 4-Hydroxybutyric acid, diTMS Butanoic acid, 4-hydroxy, bis-TMS 4-Hydroxybutyric acid, TMS Butanoic acid, 4-hydroxy, TMS 4-Hydroxybutanoic acid, 2tms derivative |
| Inchi: | InChI=1S/C10H24O3Si2/c1-14(2,3)12-9-7-8-10(11)13-15(4,5)6/h7-9H2,1-6H3 |
| InchiKey: | JQUWWJZPEOMMSB-UHFFFAOYSA-N |
| Formula: | C10H24O3Si2 |
| SMILES: | C[Si](C)(C)OCCCC(=O)O[Si](C)(C)C |
| Mol. weight [g/mol]: | 248.47 |
| CAS: | 55133-95-4 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|------|----------------|
| log10ws | 1.94 | | Crippen Method |
| logp | 2.996 | | Crippen Method |
| rinpol | 1230.00 | | NIST Webbook |
| rinpol | 1238.00 | | NIST Webbook |
| rinpol | 1246.00 | | NIST Webbook |
| rinpol | 1246.00 | | NIST Webbook |
| rinpol | 1230.40 | | NIST Webbook |
| rinpol | 1230.00 | | NIST Webbook |
| rinpol | 1234.00 | | NIST Webbook |
| rinpol | 1230.40 | | NIST Webbook |

Sources

| | |
|------------------------|---|
| Crippen Method: | https://www.chemeo.com/doc/models/crippen_log10ws |
| NIST Webbook: | http://webbook.nist.gov/cgi/cbook.cgi?ID=C55133954&Units=SI |
| Crippen Method: | http://pubs.acs.org/doi/abs/10.1021/ci9903071 |

Legend

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

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