

Pentanoic acid, 2-[(trimethylsilyl)oxy]-, trimethylsilyl ester

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| Other names: | 2-Trimethylsiloxyvaleric acid, trimethylsilyl ester 2-Hydroxyvaleric acid, di-TMS 2-Hydroxyvaleric acid, bis-TMS 2-Hydroxyvaleric acid, TMS |
| Inchi: | InChI=1S/C11H26O3Si2/c1-8-9-10(13-15(2,3)4)11(12)14-16(5,6)7/h10H,8-9H2,1-7H3 |
| InchiKey: | ATDLRMVSNYEHLG-UHFFFAOYSA-N |
| Formula: | C11H26O3Si2 |
| SMILES: | CCCC(O[Si](C)(C)C)C(=O)O[Si](C)(C)C |
| Mol. weight [g/mol]: | 262.49 |
| CAS: | 55887-46-2 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|------|----------------|
| log10ws | 1.41 | | Crippen Method |
| logp | 3.385 | | Crippen Method |
| rinpol | 1207.00 | | NIST Webbook |
| rinpol | 1199.00 | | NIST Webbook |
| rinpol | 1207.00 | | NIST Webbook |
| rinpol | 1212.00 | | NIST Webbook |
| rinpol | 1207.00 | | NIST Webbook |
| rinpol | 1199.00 | | NIST Webbook |

Sources

| | |
|------------------------|---|
| NIST Webbook: | http://webbook.nist.gov/cgi/cbook.cgi?ID=C55887462&Units=SI |
| Crippen Method: | http://pubs.acs.org/doi/abs/10.1021/ci990307I |
| Crippen Method: | https://www.chemeo.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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