# 2-Phosphonobutanoic acid, tristrimethylsilyl; ester

**Other names:** Trimethylsilyl 2-(bis[(trimethylsilyl)oxy]phosphoryl)butanoate
2-Phosphonobutyric acid, tri-TMS
**Inchi:** InChI=1S/C13H33O5PSi3/c1-11-12(13(14)16-20(2,3)4)19(15,17-21(5,6)7)18-22(8,9)10/h
**InchiKey:** HAWKAMOJPQTGNQ-UHFFFAOYSA-N
**Formula:** C13H33O5PSi3
**SMILES:** CCC(C(=O)O[Si](C)(C)C)P(=O)(O[Si](C)(C)C)O[Si](C)(C)C
**Mol. weight [g/mol]:** 384.63
**CAS:** 959220-68-9

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| log10ws | 1.16 | | Crippen Method |
| logp | 5.039 | | Crippen Method |
| rinpol | 1557.00 | | NIST Webbook |
| rinpol | 1557.00 | | NIST Webbook |

## Sources

**Crippen Method:** http://pubs.acs.org/doi/abs/10.1021/ci990307l
**Crippen Method:** https://www.chemeo.com/doc/models/crippen_log10ws
**NIST Webbook:** http://webbook.nist.gov/cgi/cbook.cgi?ID=C959220689&Units=SI

## Legend

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

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