

# Phenaceturic acid, tert-butyldimethylsilyl ester

**Other names:** tert-Butyl(dimethyl)silyl N-(phenylacetyl)glycinate

Phenaceturic acid, tbdms derivative

**Inchi:** InChI=1S/C16H25NO3Si/c1-16(2,3)21(4,5)20-15(19)12-17-14(18)11-13-9-7-6-8-10-13/h

**InchiKey:** BQEYXUXCTREUJK-UHFFFAOYSA-N

**Formula:** C16H25NO3Si

**SMILES:** CC(C)(C)[Si](C)(C)OC(=O)CNC(=O)Cc1ccccc1

**Mol. weight [g/mol]:** 307.46

## Physical Properties

| Property code | Value   | Unit | Source         |
|---------------|---------|------|----------------|
| log10ws       | -1.50   |      | Crippen Method |
| logp          | 2.894   |      | Crippen Method |
| rinpola       | 2146.30 |      | NIST Webbook   |
| rinpola       | 2146.30 |      | NIST Webbook   |

## Sources

**Crippen Method:** <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

**Crippen Method:** [https://www.cheméo.com/doc/models/crippen\\_log10ws](https://www.cheméo.com/doc/models/crippen_log10ws)

**NIST Webbook:** <http://webbook.nist.gov/cgi/cbook.cgi?ID=U333162&Units=SI>

## Legend

**log10ws:** Log10 of Water solubility in mol/l

**logp:** Octanol/Water partition coefficient

**rinpola:** Non-polar retention indices

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