

# Benzoic acid, 4-(1-trimethylsilyloxy)-2-(pyrrolidin-1-yl)butyl-, trimethylsilyl ester

Other names: 4-(1-methyl- $\alpha$ »-pyrrolidinobutyrophenone-M (carboxy-dihydro-) diTMS

Inchi: InChI=1S/C21H37NO3Si2/c1-8-19(22-15-9-10-16-22)20(24-26(2,3)4)17-11-13-18(14-12-

InchiKey: GHSNXQLJVMPLZLH-UHFFFAOYSA-N

Formula: C<sub>21</sub>H<sub>37</sub>NO<sub>3</sub>Si<sub>2</sub>

SMILES: CCC(C(O[Si](C)(C)C)c1ccc(C(=O)O[Si](C)(C)C)cc1)N1CCCC1

Mol. weight [g/mol]: 407.69

## Physical Properties

| Property code | Value   | Unit | Source         |
|---------------|---------|------|----------------|
| log10ws       | -1.35   |      | Crippen Method |
| logp          | 5.445   |      | Crippen Method |
| rinpol        | 2140.00 |      | NIST Webbook   |
| rinpol        | 2140.00 |      | NIST Webbook   |

## Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>

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=U360391&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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