

# Pentanoic acid, 4-methyl-, tert-butyldimethylsilyl ester

|                      |                                                                           |
|----------------------|---------------------------------------------------------------------------|
| Other names:         | tert-Butyl(dimethyl)silyl 4-methylpentanoate                              |
| Inchi:               | InChI=1S/C12H26O2Si/c1-10(2)8-9-11(13)14-15(6,7)12(3,4)5/h10H,8-9H2,1-7H3 |
| InchiKey:            | KCUZKZNIAAGBOY-UHFFFAOYSA-N                                               |
| Formula:             | C12H26O2Si                                                                |
| SMILES:              | CC(C)CCC(=O)O[Si](C)(C)C(C)(C)C                                           |
| Mol. weight [g/mol]: | 230.42                                                                    |

## Physical Properties

| Property code | Value   | Unit | Source             |
|---------------|---------|------|--------------------|
| ie            | 9.62    | eV   | Cheméo Relay (1.0) |
| log10ws       | -3.29   |      | Cheméo Relay (1.0) |
| logp          | 3.971   |      | Crippen Method     |
| rinpol        | 1250.10 |      | NIST Webbook       |
| rinpol        | 1250.10 |      | NIST Webbook       |
| tb            | 483.40  | K    | Cheméo Relay (1.0) |
| tf            | 249.76  | K    | Cheméo Relay (1.0) |

## Sources

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

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C959108908&Units=SI>

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

## Legend

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

**tb:** Normal Boiling Point Temperature

**tf:** Normal melting (fusion) point

Latest version available from:

<https://www.cheméo.com/cid/64-689-7/Pentanoic-acid-4-methyl-tert-butyldimethylsilyl-ester.pdf>

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