

# TRIMETHYL(PHENYLTHIOMETHYL)SILANE

|                      |                                                                        |
|----------------------|------------------------------------------------------------------------|
| Other names:         | (Phenylthiomethyl)trimethylsilane<br>Trimethyl(phenylthio)methylsilane |
| Inchi:               | InChI=1S/C10H16SSi/c1-12(2,3)9-11-10-7-5-4-6-8-10/h4-8H,9H2,1-3H3      |
| InchiKey:            | UOQDIMYVQSHALM-UHFFFAOYSA-N                                            |
| Formula:             | C10H16SSi                                                              |
| SMILES:              | C[Si](C)(C)CSc1ccccc1                                                  |
| Mol. weight [g/mol]: | 196.39                                                                 |

## Physical Properties

| Property code | Value       | Unit   | Source                   |
|---------------|-------------|--------|--------------------------|
| hf            | -74.99      | kJ/mol | Cheméo Relay (1.0)       |
| hvap          | 60.59       | kJ/mol | Cheméo Relay (1.0)       |
| ie            | 7.81 ± 0.05 | eV     | NIST Webbook             |
| log10ws       | -4.40       |        | Cheméo Relay (1.0)       |
| logp          | 3.656       |        | Crippen Method           |
| pc            | 2263.40     | kPa    | Cheméo Relay (1.0, beta) |
| tb            | 520.51      | K      | Cheméo Relay (1.0)       |

## Sources

|                           |                                                                                                                                               |
|---------------------------|-----------------------------------------------------------------------------------------------------------------------------------------------|
| NIST Webbook:             | <a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C17873084&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C17873084&amp;Units=SI</a> |
| Crippen Method:           | <a href="http://pubs.acs.org/doi/abs/10.1021/ci990307l">http://pubs.acs.org/doi/abs/10.1021/ci990307l</a>                                     |
| Crippen Method:           | <a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>                             |
| Cheméo Relay (1.0):       |                                                                                                                                               |
| Cheméo Relay (1.0, beta): |                                                                                                                                               |

## Legend

|       |                                                 |
|-------|-------------------------------------------------|
| hf:   | Enthalpy of formation at standard conditions    |
| hvap: | Enthalpy of vaporization at standard conditions |
| ie:   | Ionization energy                               |

|                 |                                     |
|-----------------|-------------------------------------|
| <b>log10ws:</b> | Log10 of Water solubility in mol/l  |
| <b>logp:</b>    | Octanol/Water partition coefficient |
| <b>pc:</b>      | Critical Pressure                   |
| <b>tb:</b>      | Normal Boiling Point Temperature    |

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