

# Trifluorophenylsilane

|                      |                                                 |
|----------------------|-------------------------------------------------|
| Other names:         | Phenyl trifluorosilane                          |
| Inchi:               | InChI=1S/C6H5F3Si/c7-10(8,9)6-4-2-1-3-5-6/h1-5H |
| InchiKey:            | KGWNTTHHPMKEAIK-UHFFFAOYSA-N                    |
| Formula:             | C6H5F3Si                                        |
| SMILES:              | F[Si](F)(F)c1ccccc1                             |
| Mol. weight [g/mol]: | 162.18                                          |
| CAS:                 | 368-47-8                                        |

## Physical Properties

| Property code | Value | Unit | Source         |
|---------------|-------|------|----------------|
| ie            | 10.23 | eV   | NIST Webbook   |
| log10ws       | -4.19 |      | Crippen Method |
| logp          | 1.741 |      | Crippen Method |

## Temperature Dependent Properties

| Property code | Value | Unit   | Temperature [K] | Source       |
|---------------|-------|--------|-----------------|--------------|
| hvapt         | 40.10 | kJ/mol | 306.50          | NIST Webbook |

## Correlations

| Information                 | Value                         |
|-----------------------------|-------------------------------|
| Property code               | pvap                          |
| Equation                    | $\ln(P_{vp}) = A + B/(T + C)$ |
| Coeff. A                    | 1.74100e+01                   |
| Coeff. B                    | -5.11398e+03                  |
| Coeff. C                    | 2.51400e+01                   |
| Temperature range (K), min. | 263.00                        |
| Temperature range (K), max. | 397.55                        |

# Sources

|                                             |                                                                                                                                                                                         |
|---------------------------------------------|-----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| <b>Crippen Method:</b>                      | <a href="http://pubs.acs.org/doi/abs/10.1021/ci990307l">http://pubs.acs.org/doi/abs/10.1021/ci990307l</a>                                                                               |
| <b>Crippen Method:</b>                      | <a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>                                                                       |
| <b>NIST Webbook:</b>                        | <a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C368478&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C368478&amp;Units=SI</a>                                               |
| <b>The Yaws Handbook of Vapor Pressure:</b> | <a href="https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure">https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure</a> |

## Legend

|                 |                                                 |
|-----------------|-------------------------------------------------|
| <b>hvapt:</b>   | Enthalpy of vaporization at a given temperature |
| <b>ie:</b>      | Ionization energy                               |
| <b>log10ws:</b> | Log10 of Water solubility in mol/l              |
| <b>logp:</b>    | Octanol/Water partition coefficient             |
| <b>pvap:</b>    | Vapor pressure                                  |

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