

# Phosphine, triphenyl-

|                             |   |
|-----------------------------|---|
| <b>Other names:</b>         | NSC 10<br>NSC 215203<br>PP 360<br>Phosphorus triphenyl<br>Trifenylfosfin<br>Triphenylphosphane<br>Triphenylphosphide<br>Triphenylphosphine<br>Triphenylphosphorus |
| <b>Inchi:</b>               | InChI=1S/C18H15P/c1-4-10-16(11-5-1)19(17-12-6-2-7-13-17)18-14-8-3-9-15-18/h1-15H  |
| <b>InchiKey:</b>            | RIOQSEWOXXDEQQ-UHFFFAOYSA-N   |
| <b>Formula:</b>             | C18H15P   |
| <b>SMILES:</b>              | c1ccc(P(c2ccccc2)c2ccccc2)cc1   |
| <b>Mol. weight [g/mol]:</b> | 262.29  |
| <b>CAS:</b>                 | 603-35-0  |

## Physical Properties

| Property code | Value         | Unit   | Source         |
|---------------|---------------|--------|----------------|
| affp          | 972.80        | kJ/mol | NIST Webbook   |
| basg          | 940.40        | kJ/mol | NIST Webbook   |
| hsub          | 96.20 ± 8.40  | kJ/mol | NIST Webbook   |
| hsub          | 113.20 ± 3.00 | kJ/mol | NIST Webbook   |
| ie            | 7.37 ± 0.01   | eV     | NIST Webbook   |
| ie            | 7.36 ± 0.05   | eV     | NIST Webbook   |
| ie            | 8.20 ± 0.05   | eV     | NIST Webbook   |
| ie            | 7.83          | eV     | NIST Webbook   |
| ie            | 7.80 ± 0.05   | eV     | NIST Webbook   |
| ie            | 7.97          | eV     | NIST Webbook   |
| ie            | 7.80          | eV     | NIST Webbook   |
| ie            | 7.92          | eV     | NIST Webbook   |
| ie            | 7.44 ± 0.05   | eV     | NIST Webbook   |
| ie            | 7.85 ± 0.05   | eV     | NIST Webbook   |
| log10ws       | -13.68        |        | Crippen Method |
| logp          | 3.445         |        | Crippen Method |
| mcvol         | 213.660       | ml/mol | McGowan Method |
| tf            | 353.70 ± 0.50 | K      | NIST Webbook   |
| tf            | 354.40 ± 0.50 | K      | NIST Webbook   |

|    |               |   |   |
|----|---------------|---|---|
| tf | 352.65        | K | Solubilities of Phenylphosphinic Acid, Hydroxymethylphenylphosphinic Acid, p-Methoxyphenylphosphinic Acid, p-Methoxyphenylhydroxymethylphosphinic Acid, Triphenylphosphine, Tri(p-methoxyphenyl)phosphine, and Tri(p-methoxyphenyl)phosphine Oxide in Selected Solvents |
| tf | 347.85 ± 0.50 | K | NIST Webbook  |
| tf | 350.40 ± 1.00 | K | NIST Webbook  |

## Temperature Dependent Properties

| Property code | Value         | Unit    | Temperature [K] | Source       |
|---------------|---------------|---------|-----------------|--------------|
| cps           | 312.50        | J/mol×K | 298.50          | NIST Webbook |
| hfust         | 19.69         | kJ/mol  | 354.40          | NIST Webbook |
| hfust         | 19.69         | kJ/mol  | 354.40          | NIST Webbook |
| hfust         | 19.69         | kJ/mol  | 354.40          | NIST Webbook |
| hsubt         | 109.20 ± 1.10 | kJ/mol  | 350.00          | NIST Webbook |
| hvapt         | 71.20         | kJ/mol  | 571.50          | NIST Webbook |
| hvapt         | 91.00 ± 2.00  | kJ/mol  | 378.00          | NIST Webbook |
| sfust         | 55.56         | J/mol×K | 354.40          | NIST Webbook |

## Correlations

| Information                 | Value                                 |
|-----------------------------|---------------------------------------|
| Property code               | pvap                                  |
| Equation                    | $\ln(P_{\text{vap}}) = A + B/(T + C)$ |
| Coeff. A                    | 1.57798e+01                           |
| Coeff. B                    | -6.25733e+03                          |
| Coeff. C                    | -8.95290e+01                          |
| Temperature range (K), min. | 493.15                                |
| Temperature range (K), max. | 687.15                                |

# Sources

|  |   |
|--|---|
| <b>Solubilities of Triphenylphosphine in Ethanol, 2-Propanol, Acetone, Benzene, and Toluene Method:</b>  | <a href="https://www.doi.org/10.1021/je060350m">https://www.doi.org/10.1021/je060350m</a><br><a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>  |
| <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>NIST Webbook:</b>   | <a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C603350&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C603350&amp;Units=SI</a>   |
| <b>Solubilities of Phenylphosphinic Acid, Hydroxymethylphenylphosphinic Acid, S-methoxyphenylphosphinic Acid, Thermodynamic Modeling of S-methoxyphenylphosphinic Acid, Yaws Handbook of Vapor Pressure, Mixtures from Phosphine, and Crippen Method: The Chemistry of adducts of some bivalent transition metal bromides with triphenylphosphine:</b> | <a href="https://www.doi.org/10.1021/je050377q">https://www.doi.org/10.1021/je050377q</a><br><a href="https://www.doi.org/10.1021/acs.jced.7b00245">https://www.doi.org/10.1021/acs.jced.7b00245</a><br><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><br><a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a><br><a href="https://www.doi.org/10.1016/j.tca.2005.06.016">https://www.doi.org/10.1016/j.tca.2005.06.016</a> |

## Legend

|                 |   |
|-----------------|---|
| <b>affp:</b>    | Proton affinity                                 |
| <b>basg:</b>    | Gas basicity                                    |
| <b>cps:</b>     | Solid phase heat capacity                       |
| <b>hfust:</b>   | Enthalpy of fusion at a given temperature       |
| <b>hsub:</b>    | Enthalpy of sublimation at standard conditions  |
| <b>hsubt:</b>   | Enthalpy of sublimation at a given temperature  |
| <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>mcvol:</b>   | McGowan's characteristic volume                 |
| <b>pvap:</b>    | Vapor pressure                                  |
| <b>sfust:</b>   | Entropy of fusion at a given temperature        |
| <b>tf:</b>      | Normal melting (fusion) point                   |

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