

# 5-Phenyl-2,4-pentadienophenone

|                             |  |
|-----------------------------|--|
| <b>Other names:</b>         | Cinnamylideneacetophenone<br>«alpha»-Cinnamylideneacetophenone<br>2,4-Pentadien-1-one, 1,5-diphenyl-<br>5-phenylpenta-2,4-dienophenone |
| <b>Inchi:</b>               | InChI=1S/C17H14O/c18-17(16-12-5-2-6-13-16)14-8-7-11-15-9-3-1-4-10-15/h1-14H/b11-   |
| <b>InchiKey:</b>            | QONKLJMPKWQQFG-HPIZBCMHTSA-N   |
| <b>Formula:</b>             | C17H14O  |
| <b>SMILES:</b>              | O=C(C=CC=Cc1ccccc1)c1ccccc1  |
| <b>Mol. weight [g/mol]:</b> | 234.29   |
| <b>CAS:</b>                 | 614-57-3   |

## Physical Properties

| Property code | Value   | Unit                 | Source         |
|---------------|---------|----------------------|----------------|
| gf            | 348.60  | kJ/mol               | Joback Method  |
| hf            | 200.71  | kJ/mol               | Joback Method  |
| hfus          | 29.87   | kJ/mol               | Joback Method  |
| hvap          | 64.65   | kJ/mol               | Joback Method  |
| log10ws       | -4.88   |                      | Crippen Method |
| logp          | 4.139   |                      | Crippen Method |
| mcvol         | 195.840 | ml/mol               | McGowan Method |
| pc            | 2448.32 | kPa                  | Joback Method  |
| tb            | 703.91  | K                    | Joback Method  |
| tc            | 954.96  | K                    | Joback Method  |
| tf            | 373.96  | K                    | Joback Method  |
| vc            | 0.738   | m <sup>3</sup> /kmol | Joback Method  |

## Temperature Dependent Properties

| Property code | Value  | Unit    | Temperature [K] | Source        |
|---------------|--------|---------|-----------------|---------------|
| cpg           | 498.70 | J/molxK | 703.91          | Joback Method |
| cpg           | 565.84 | J/molxK | 913.11          | Joback Method |
| cpg           | 554.49 | J/molxK | 871.27          | Joback Method |
| cpg           | 542.24 | J/molxK | 829.43          | Joback Method |
| cpg           | 528.96 | J/molxK | 787.59          | Joback Method |

|       |           |         |        |               |
|-------|-----------|---------|--------|---------------|
| cpg   | 514.49    | J/molxK | 745.75 | Joback Method |
| cpg   | 576.44    | J/molxK | 954.96 | Joback Method |
| dvisc | 0.0001044 | Paxs    | 703.91 | Joback Method |
| dvisc | 0.0001357 | Paxs    | 648.92 | Joback Method |
| dvisc | 0.0001851 | Paxs    | 593.93 | Joback Method |
| dvisc | 0.0002691 | Paxs    | 538.93 | Joback Method |
| dvisc | 0.0004258 | Paxs    | 483.94 | Joback Method |
| dvisc | 0.0007579 | Paxs    | 428.95 | Joback Method |
| dvisc | 0.0015983 | Paxs    | 373.96 | Joback Method |

## Sources

|                        |   |
|------------------------|---|
| <b>Joback Method:</b>  | <a href="https://en.wikipedia.org/wiki/Joback_method">https://en.wikipedia.org/wiki/Joback_method</a>                                     |
| <b>McGowan Method:</b> | <a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>                     |
| <b>NIST Webbook:</b>   | <a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C614573&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C614573&amp;Units=SI</a> |
| <b>Crippen Method:</b> | <a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</a>                                 |
| <b>Crippen Method:</b> | <a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>                         |

## Legend

|                 |   |
|-----------------|---|
| <b>cpg:</b>     | Ideal gas heat capacity                         |
| <b>dvisc:</b>   | Dynamic viscosity                               |
| <b>gf:</b>      | Standard Gibbs free energy of formation         |
| <b>hf:</b>      | Enthalpy of formation at standard conditions    |
| <b>hfus:</b>    | Enthalpy of fusion at standard conditions       |
| <b>hvap:</b>    | Enthalpy of vaporization at standard conditions |
| <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>pc:</b>      | Critical Pressure                               |
| <b>tb:</b>      | Normal Boiling Point Temperature                |
| <b>tc:</b>      | Critical Temperature                            |
| <b>tf:</b>      | Normal melting (fusion) point                   |
| <b>vc:</b>      | Critical Volume                                 |

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