

# Ethanone, 1-[1,1'-biphenyl]-4-yl-

|                      |                                                                                                                                                                                                                                                                                                                                                                                                                        |
|----------------------|------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| Other names:         | Acetophenone, 4'-phenyl-<br>p-Phenylacetophenone<br>Ketone, 4-biphenylyl methyl<br>4-Acetylbiphenyl<br>4-Biphenylyl methyl ketone<br>4-Phenylacetophenone<br>4'-Phenylacetophenone<br>4-Diphenyl methyl ketone<br>p-Biphenylyl methyl ketone<br>4-Acetylbibenzyl<br>p-Acetylbiphenyl<br>Methyl 4-biphenylyl ketone<br>1-Acetyl-4-phenylbenzene<br>4-Phenyl-acetophenon<br>1,1'-Biphenyl-4-yl methyl ketone<br>NSC 1875 |
| Inchi:               | InChI=1S/C14H12O/c1-11(15)12-7-9-14(10-8-12)13-5-3-2-4-6-13/h2-10H,1H3                                                                                                                                                                                                                                                                                                                                                 |
| InchiKey:            | QCZZSANNLWPGEA-UHFFFAOYSA-N                                                                                                                                                                                                                                                                                                                                                                                            |
| Formula:             | C14H12O                                                                                                                                                                                                                                                                                                                                                                                                                |
| SMILES:              | CC(=O)c1ccc(-c2ccccc2)cc1                                                                                                                                                                                                                                                                                                                                                                                              |
| Mol. weight [g/mol]: | 196.24                                                                                                                                                                                                                                                                                                                                                                                                                 |
| CAS:                 | 92-91-1                                                                                                                                                                                                                                                                                                                                                                                                                |

## Physical Properties

| Property code | Value         | Unit   | Source         |
|---------------|---------------|--------|----------------|
| gf            | 153.27        | kJ/mol | Joback Method  |
| hf            | 16.72         | kJ/mol | Joback Method  |
| hfus          | 21.31         | kJ/mol | Joback Method  |
| hvap          | 58.72         | kJ/mol | Joback Method  |
| log10ws       | -4.73         |        | Crippen Method |
| logp          | 3.556         |        | Crippen Method |
| mcvol         | 162.170       | ml/mol | McGowan Method |
| pc            | 2915.53       | kPa    | Joback Method  |
| tb            | 599.20        | K      | NIST Webbook   |
| tb            | 599.00 ± 1.00 | K      | NIST Webbook   |
| tc            | 879.64        | K      | Joback Method  |
| tf            | 393.50 ± 0.50 | K      | NIST Webbook   |

|    |       |                      |               |
|----|-------|----------------------|---------------|
| vc | 0.610 | m <sup>3</sup> /kmol | Joback Method |
|----|-------|----------------------|---------------|

## Temperature Dependent Properties

| Property code | Value     | Unit    | Temperature [K] | Source        |
|---------------|-----------|---------|-----------------|---------------|
| cpg           | 390.09    | J/mol×K | 631.93          | Joback Method |
| cpg           | 456.04    | J/mol×K | 838.35          | Joback Method |
| cpg           | 445.06    | J/mol×K | 797.07          | Joback Method |
| cpg           | 433.04    | J/mol×K | 755.78          | Joback Method |
| cpg           | 419.92    | J/mol×K | 714.50          | Joback Method |
| cpg           | 405.63    | J/mol×K | 673.21          | Joback Method |
| cpg           | 466.07    | J/mol×K | 879.64          | Joback Method |
| dvisc         | 0.0001874 | Pa×s    | 631.93          | Joback Method |
| dvisc         | 0.0002356 | Pa×s    | 587.08          | Joback Method |
| dvisc         | 0.0003075 | Pa×s    | 542.23          | Joback Method |
| dvisc         | 0.0004210 | Pa×s    | 497.38          | Joback Method |
| dvisc         | 0.0006136 | Pa×s    | 452.53          | Joback Method |
| dvisc         | 0.0009716 | Pa×s    | 407.68          | Joback Method |
| dvisc         | 0.0017236 | Pa×s    | 362.83          | Joback Method |

## Pressure Dependent Properties

| Property code | Value         | Unit | Pressure [kPa] | Source       |
|---------------|---------------|------|----------------|--------------|
| tbrp          | 408.00 ± 5.00 | K    | 0.40           | NIST Webbook |

## Sources

|                 |                                                                                                                                         |
|-----------------|-----------------------------------------------------------------------------------------------------------------------------------------|
| Crippen Method: | <a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>                       |
| Joback Method:  | <a href="https://en.wikipedia.org/wiki/Joback_method">https://en.wikipedia.org/wiki/Joback_method</a>                                   |
| McGowan Method: | <a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>                   |
| NIST Webbook:   | <a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C92911&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C92911&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>                               |

# 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>tbrp:</b>    | Boiling point at reduced pressure               |
| <b>tc:</b>      | Critical Temperature                            |
| <b>tf:</b>      | Normal melting (fusion) point                   |
| <b>vc:</b>      | Critical Volume                                 |

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