

# Methanone, [4-(1-methylethyl)phenyl]phenyl-

|                             |  |
|-----------------------------|--|
| <b>Other names:</b>         | Benzophenone, 4-isopropyl-<br>p-Isopropylbenzophenone<br>4-Isopropylbenzophenone |
| <b>Inchi:</b>               | InChI=1S/C16H16O/c1-12(2)13-8-10-15(11-9-13)16(17)14-6-4-3-5-7-14/h3-12H,1-2H3   |
| <b>InchiKey:</b>            | CKFPWZPBRHQASN-UHFFFAOYSA-N  |
| <b>Formula:</b>             | C16H16O  |
| <b>SMILES:</b>              | CC(C)c1ccc(C(=O)c2ccccc2)cc1   |
| <b>Mol. weight [g/mol]:</b> | 224.30   |
| <b>CAS:</b>                 | 18864-76-1   |

## Physical Properties

| Property code | Value           | Unit                 | Source         |
|---------------|-----------------|----------------------|----------------|
| chl           | -8464.00 ± 2.00 | kJ/mol               | NIST Webbook   |
| gf            | 167.67          | kJ/mol               | Joback Method  |
| hf            | -29.84          | kJ/mol               | Joback Method  |
| hfl           | -119.00         | kJ/mol               | NIST Webbook   |
| hfus          | 22.96           | kJ/mol               | Joback Method  |
| hvap          | 62.78           | kJ/mol               | Joback Method  |
| log10ws       | -4.61           |                      | Crippen Method |
| logp          | 4.041           |                      | Crippen Method |
| mcvol         | 190.350         | ml/mol               | McGowan Method |
| pc            | 2412.37         | kPa                  | Joback Method  |
| tb            | 677.25          | K                    | Joback Method  |
| tc            | 919.42          | K                    | Joback Method  |
| tf            | 370.37          | K                    | Joback Method  |
| vc            | 0.716           | m <sup>3</sup> /kmol | Joback Method  |

## Temperature Dependent Properties

| Property code | Value  | Unit    | Temperature [K] | Source        |
|---------------|--------|---------|-----------------|---------------|
| cpg           | 492.14 | J/mol×K | 677.25          | Joback Method |
| cpg           | 508.98 | J/mol×K | 717.61          | Joback Method |
| cpg           | 524.51 | J/mol×K | 757.97          | Joback Method |
| cpg           | 538.79 | J/mol×K | 798.34          | Joback Method |

|       |           |         |        |               |
|-------|-----------|---------|--------|---------------|
| cpg   | 551.91    | J/mol×K | 838.70 | Joback Method |
| cpg   | 563.94    | J/mol×K | 879.06 | Joback Method |
| cpg   | 574.96    | J/mol×K | 919.42 | Joback Method |
| dvisc | 0.0019166 | Paxs    | 370.37 | Joback Method |
| dvisc | 0.0009580 | Paxs    | 421.52 | Joback Method |
| dvisc | 0.0005564 | Paxs    | 472.66 | Joback Method |
| dvisc | 0.0003593 | Paxs    | 523.81 | Joback Method |
| dvisc | 0.0002508 | Paxs    | 574.96 | Joback Method |
| dvisc | 0.0001857 | Paxs    | 626.10 | Joback Method |
| dvisc | 0.0001439 | Paxs    | 677.25 | Joback Method |

## Sources

|                        |   |
|------------------------|---|
| <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>                             |
| <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=C18864761&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C18864761&amp;Units=SI</a> |

## Legend

|                 |   |
|-----------------|---|
| <b>chl:</b>     | Standard liquid enthalpy of combustion                    |
| <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>hfl:</b>     | Liquid phase 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   |

Latest version available from:

<https://www.chemeo.com/cid/16-722-2/Methanone-4-1-methylethyl-phenyl-phenyl.pdf>

Generated by Cheméo on 2024-04-18 22:09:16.659825623 +0000 UTC m=+15767405.580402958.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.