

# Alpha,alpha-diphenyl acetophenone

|                      |                                                                                  |
|----------------------|----------------------------------------------------------------------------------|
| Inchi:               | InChI=1S/C20H16O/c21-20(19-9-5-2-6-10-19)15-16-11-13-18(14-12-16)17-7-3-1-4-8-17 |
| InchiKey:            | HZXXIQLDHPWKLO-UHFFFAOYSA-N                                                      |
| Formula:             | C20H16O                                                                          |
| SMILES:              | O=C(Cc1ccc(-c2ccccc2)cc1)c1ccccc1                                                |
| Mol. weight [g/mol]: | 272.34                                                                           |
| CAS:                 | 27644-00-4                                                                       |

## Physical Properties

| Property code | Value   | Unit    | Source         |
|---------------|---------|---------|----------------|
| gf            | 316.20  | kJ/mol  | Joback Method  |
| hf            | 129.41  | kJ/mol  | Joback Method  |
| hfus          | 30.89   | kJ/mol  | Joback Method  |
| hvap          | 74.35   | kJ/mol  | Joback Method  |
| log10ws       | -6.35   |         | Crippen Method |
| logp          | 4.779   |         | Crippen Method |
| mcvol         | 222.950 | ml/mol  | McGowan Method |
| pc            | 2274.07 | kPa     | Joback Method  |
| tb            | 795.89  | K       | Joback Method  |
| tc            | 1057.67 | K       | Joback Method  |
| tf            | 456.87  | K       | Joback Method  |
| vc            | 0.838   | m3/kmol | Joback Method  |

## Temperature Dependent Properties

| Property code | Value     | Unit    | Temperature [K] | Source        |
|---------------|-----------|---------|-----------------|---------------|
| cpg           | 618.55    | J/mol×K | 795.89          | Joback Method |
| cpg           | 634.55    | J/mol×K | 839.52          | Joback Method |
| cpg           | 649.06    | J/mol×K | 883.15          | Joback Method |
| cpg           | 662.20    | J/mol×K | 926.78          | Joback Method |
| cpg           | 674.11    | J/mol×K | 970.41          | Joback Method |
| cpg           | 684.92    | J/mol×K | 1014.04         | Joback Method |
| cpg           | 694.77    | J/mol×K | 1057.67         | Joback Method |
| dvisc         | 0.0010319 | Pa×s    | 456.87          | Joback Method |
| dvisc         | 0.0005666 | Pa×s    | 513.37          | Joback Method |

|       |           |      |        |               |
|-------|-----------|------|--------|---------------|
| dvisc | 0.0003503 | Pa×s | 569.88 | Joback Method |
| dvisc | 0.0002363 | Pa×s | 626.38 | Joback Method |
| dvisc | 0.0001701 | Pa×s | 682.88 | Joback Method |
| dvisc | 0.0001287 | Pa×s | 739.39 | Joback Method |
| dvisc | 0.0001014 | Pa×s | 795.89 | Joback Method |

## Sources

|                        |                                                                                                                                               |
|------------------------|-----------------------------------------------------------------------------------------------------------------------------------------------|
| <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=C27644004&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C27644004&amp;Units=SI</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>                                     |

## 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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