# 3-hydroxy-4-phenyl-2-butanone

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|---|---|
| **Other names:** | 4-phenyl-3-hydroxybutan-2-one |
| | 2-Hydroxy-1-phenylbutan-3-one |
| | 2-Butanone, 3-hydroxy-4-phenyl |
| | 3-hydroxy-4-phenylbutan-2-one |
| **Inchi:** | InChI=1S/C10H12O2/c1-8(11)10(12)7-9-5-3-2-4-6-9/h2-6,10,12H,7H2,1H3 |
| **InchiKey:** | QBCUUJGHWFKMDC-UHFFFAOYSA-N |
| **Formula:** | C10H12O2 |
| **SMILES:** | CC(=O)C(O)Cc1ccccc1 |
| **Mol. weight [g/mol]:** | 164.20 |
| **CAS:** | 5355-63-5 |

# Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -122.45 | kJ/mol | Joback Method |
| hf | -283.29 | kJ/mol | Joback Method |
| hfus | 17.86 | kJ/mol | Joback Method |
| hvap | 63.17 | kJ/mol | Joback Method |
| log10ws | -1.77 | | Crippen Method |
| logp | 1.179 | | Crippen Method |
| mcvol | 135.440 | ml/mol | McGowan Method |
| pc | 3526.27 | kPa | Joback Method |
| rinpol | 1348.00 | | NIST Webbook |
| rinpol | 1362.00 | | NIST Webbook |
| rinpol | 1360.00 | | NIST Webbook |
| rinpol | 1375.00 | | NIST Webbook |
| rinpol | 1348.00 | | NIST Webbook |
| rinpol | 1348.00 | | NIST Webbook |
| ripol | 2260.00 | | NIST Webbook |
| ripol | 2259.00 | | NIST Webbook |
| ripol | 2260.00 | | NIST Webbook |
| ripol | 2256.00 | | NIST Webbook |
| tb | 600.49 | K | Joback Method |
| tc | 804.72 | K | Joback Method |
| tf | 324.63 | K | Joback Method |
| vc | 0.506 | m3/kmol | Joback Method |

# Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 328.11 | J/mol×K | 600.49 | Joback Method |
| cpg | 339.69 | J/mol×K | 634.53 | Joback Method |
| cpg | 350.55 | J/mol×K | 668.57 | Joback Method |
| cpg | 360.71 | J/mol×K | 702.61 | Joback Method |
| cpg | 370.22 | J/mol×K | 736.64 | Joback Method |
| cpg | 379.10 | J/mol×K | 770.68 | Joback Method |
| cpg | 387.38 | J/mol×K | 804.72 | Joback Method |
| dvisc | 0.0090484 | Pa×s | 324.63 | Joback Method |
| dvisc | 0.0025745 | Pa×s | 370.61 | Joback Method |
| dvisc | 0.0009668 | Pa×s | 416.58 | Joback Method |
| dvisc | 0.0004411 | Pa×s | 462.56 | Joback Method |
| dvisc | 0.0002319 | Pa×s | 508.54 | Joback Method |
| dvisc | 0.0001356 | Pa×s | 554.51 | Joback Method |
| dvisc | 0.0000861 | Pa×s | 600.49 | Joback Method |

# Sources

**NIST Webbook:** http://webbook.nist.gov/cgi/cbook.cgi?ID=C5355635&Units=SI
**Crippen Method:** http://pubs.acs.org/doi/abs/10.1021/ci990307l
**Crippen Method:** https://www.chemeo.com/doc/models/crippen_log10ws
**Joback Method:** https://en.wikipedia.org/wiki/Joback_method
**McGowan Method:** http://link.springer.com/article/10.1007/BF02311772

# Legend

**cpg:** Ideal gas heat capacity
**dvisc:** Dynamic viscosity
**gf:** Standard Gibbs free energy of formation
**hf:** Enthalpy of formation at standard conditions
**hfus:** Enthalpy of fusion at standard conditions
**hvap:** Enthalpy of vaporization at standard conditions
**log10ws:** Log10 of Water solubility in mol/l
**logp:** Octanol/Water partition coefficient

| | |
|---|---|
| **mcvol:** | McGowan's characteristic volume |
| **pc:** | Critical Pressure |
| **rinpol:** | Non-polar retention indices |
| **ripol:** | Polar retention indices |
| **tb:** | Normal Boiling Point Temperature |
| **tc:** | Critical Temperature |
| **tf:** | Normal melting (fusion) point |
| **vc:** | Critical Volume |

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