# 3-HYDROXY-1-PHENYLPROPAN-1-ONE

**Other names:** 3-Hydroxy-1-phenylpropan-1-one
3-Hydroxypropiophenone
**Inchi:** InChI=1S/C9H10O2/c10-7-6-9(11)8-4-2-1-3-5-8/h1-5,10H,6-7H2
**InchiKey:** PQCFUZMQHVIOSM-UHFFFAOYSA-N
**Formula:** C9H10O2
**SMILES:** O=C(CCO)c1ccccc1
**Mol. weight [g/mol]:** 150.18

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| af | 0.6816 | | Cheméo Relay (1.0) |
| gf | -128.43 | kJ/mol | Joback Method |
| hf | -278.94 | kJ/mol | Cheméo Relay (1.0) |
| hfus | 18.79 | kJ/mol | Joback Method |
| hvap | 82.87 | kJ/mol | Cheméo Relay (1.0) |
| ie | 9.26 | eV | Cheméo Relay (1.0) |
| log10ws | -1.11 | | Cheméo Relay (1.0) |
| logp | 1.252 | | Crippen Method |
| mcvol | 121.350 | ml/mol | McGowan Method |
| pc | 3925.85 | kPa | Joback Method |
| rinpol | 1462.00 | | NIST Webbook |
| rinpol | 1462.00 | | NIST Webbook |
| tb | 547.06 | K | Cheméo Relay (1.0) |
| tc | 793.48 | K | Cheméo Relay (1.0) |
| tf | 312.74 | K | Cheméo Relay (1.0) |
| vc | 0.429 | m3/kmol | Cheméo Relay (1.0) |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 281.36 | J/mol×K | 578.05 | Joback Method |
| cpg | 291.87 | J/mol×K | 611.92 | Joback Method |
| cpg | 301.73 | J/mol×K | 645.78 | Joback Method |
| cpg | 310.96 | J/mol×K | 679.65 | Joback Method |

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|---|---|---|---|---|
| cpg | 319.60 | J/mol×K | 713.51 | Joback Method |
| cpg | 327.67 | J/mol×K | 747.38 | Joback Method |
| cpg | 335.20 | J/mol×K | 781.24 | Joback Method |
| dvisc | 0.0068844 | Pa×s | 328.36 | Joback Method |
| dvisc | 0.0023345 | Pa×s | 369.98 | Joback Method |
| dvisc | 0.0009851 | Pa×s | 411.59 | Joback Method |
| dvisc | 0.0004871 | Pa×s | 453.20 | Joback Method |
| dvisc | 0.0002711 | Pa×s | 494.82 | Joback Method |
| dvisc | 0.0001653 | Pa×s | 536.43 | Joback Method |
| dvisc | 0.0001082 | Pa×s | 578.05 | Joback Method |

# Sources

**McGowan Method:** http://link.springer.com/article/10.1007/BF02311772

**Crippen Method:** http://pubs.acs.org/doi/abs/10.1021/ci990307l

**Crippen Method:** https://www.chemeo.com/doc/models/crippen_log10ws

**Cheméo Relay (1.0):**

**Cheméo Relay (1.0, beta):**

**NIST Webbook:** http://webbook.nist.gov/cgi/cbook.cgi?ID=C5650419&Units=SI

**Joback Method:** https://en.wikipedia.org/wiki/Joback_method

# Legend

**af:** Acentric Factor

**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

**ie:** Ionization energy

**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

**tb:** Normal Boiling Point Temperature

**tc:** Critical Temperature

**tf:** Normal melting (fusion) point

**vc:** Critical Volume