# 2,2-DIMETHYL-3-HYDROXYPROPIONALDEHYDE

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|---|---|
| **Other names:** | 3-Hydroxypivalaldehyde |
| | Hydroxypivaldehyde |
| | Propanal, 3-hydroxy-2,2-dimethyl- |
| | 3-hydroxy-2,2-dimethylpropionaldehyde |
| **Inchi:** | InChI=1S/C5H10O2/c1-5(2,3-6)4-7/h3,7H,4H2,1-2H3 |
| **InchiKey:** | JJMOMMLADQPZNY-UHFFFAOYSA-N |
| **Formula:** | C5H10O2 |
| **SMILES:** | CC(C)(C=O)CO |
| **Mol. weight [g/mol]:** | 102.13 |

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| af | 0.5853 | | Cheméo Relay (1.0) |
| gf | -242.28 | kJ/mol | Joback Method |
| hf | -392.77 | kJ/mol | Cheméo Relay (1.0) |
| hfus | 7.67 | kJ/mol | Joback Method |
| hvap | 56.51 | kJ/mol | Cheméo Relay (1.0) |
| ie | 9.55 | eV | Cheméo Relay (1.0) |
| log10ws | 0.15 | | Cheméo Relay (1.0) |
| logp | 0.204 | | Crippen Method |
| mcvol | 88.750 | ml/mol | McGowan Method |
| pc | 4368.40 | kPa | Joback Method |
| tb | 433.95 | K | Cheméo Relay (1.0) |
| tc | 648.23 | K | Cheméo Relay (1.0) |
| tf | 307.24 | K | Cheméo Relay (1.0) |
| vc | 0.322 | m3/kmol | Cheméo Relay (1.0) |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 188.75 | J/mol×K | 451.41 | Joback Method |
| cpg | 197.18 | J/mol×K | 481.18 | Joback Method |
| cpg | 205.15 | J/mol×K | 510.94 | Joback Method |
| cpg | 212.68 | J/mol×K | 540.71 | Joback Method |

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|---|---|---|---|---|
| cpg | 219.79 | J/mol×K | 570.48 | Joback Method |
| cpg | 226.50 | J/mol×K | 600.25 | Joback Method |
| cpg | 232.84 | J/mol×K | 630.01 | Joback Method |
| dvisc | 0.0496499 | Pa×s | 251.35 | Joback Method |
| dvisc | 0.0126525 | Pa×s | 284.69 | Joback Method |
| dvisc | 0.0042947 | Pa×s | 318.04 | Joback Method |
| dvisc | 0.0017896 | Pa×s | 351.38 | Joback Method |
| dvisc | 0.0008679 | Pa×s | 384.72 | Joback Method |
| dvisc | 0.0004724 | Pa×s | 418.07 | Joback Method |
| dvisc | 0.0002813 | Pa×s | 451.41 | Joback Method |

# Pressure Dependent Properties

| Property code | Value | Unit | Pressure [kPa] | Source |
|---|---|---|---|---|
| tbrp | 354.20 | K | 0.50 | NIST Webbook |

# Sources

**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=C597319&Units=SI
**Joback Method:** https://en.wikipedia.org/wiki/Joback_method
**McGowan Method:** http://link.springer.com/article/10.1007/BF02311772

# 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

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|---|---|
| **ie:** | Ionization energy |
| **log10ws:** | Log10 of Water solubility in mol/l |
| **logp:** | Octanol/Water partition coefficient |
| **mcvol:** | McGowan's characteristic volume |
| **pc:** | Critical Pressure |
| **tb:** | Normal Boiling Point Temperature |
| **tbrp:** | Boiling point at reduced pressure |
| **tc:** | Critical Temperature |
| **tf:** | Normal melting (fusion) point |
| **vc:** | Critical Volume |