# 3,5-Dinitro-4-hydroxybenzaldehyde

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|---|---|
| **Other names:** | Benzaldehyde, 4-hydroxy-3,5-dinitro-<br>4-hydroxy-3,5-dinitrobenzaldehyde |
| **Inchi:** | InChI=1S/C7H4N2O6/c10-3-4-1-5(8(12)13)7(11)6(2-4)9(14)15/h1-3,11H |
| **InchiKey:** | DFAVWLKOYKKDFX-UHFFFAOYSA-N |
| **Formula:** | C7H4N2O6 |
| **SMILES:** | O=Cc1cc([N+](=O)[O-])c(O)c([N+](=O)[O-])c1 |
| **Mol. weight [g/mol]:** | 212.12 |
| **CAS:** | 52132-61-3 |

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -81.83 | kJ/mol | Joback Method |
| hf | -258.63 | kJ/mol | Joback Method |
| hfus | 37.94 | kJ/mol | Joback Method |
| hvap | 87.69 | kJ/mol | Joback Method |
| log10ws | -2.56 | | Crippen Method |
| logp | 1.021 | | Crippen Method |
| mcvol | 128.010 | ml/mol | McGowan Method |
| pc | 5552.58 | kPa | Joback Method |
| tb | 829.16 | K | Joback Method |
| tc | 1106.41 | K | Joback Method |
| tf | 661.05 | K | Joback Method |
| vc | 0.467 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 337.50 | J/mol×K | 829.16 | Joback Method |
| cpg | 344.40 | J/mol×K | 875.37 | Joback Method |
| cpg | 350.92 | J/mol×K | 921.58 | Joback Method |
| cpg | 357.21 | J/mol×K | 967.79 | Joback Method |
| cpg | 363.39 | J/mol×K | 1013.99 | Joback Method |
| cpg | 369.58 | J/mol×K | 1060.20 | Joback Method |
| cpg | 375.92 | J/mol×K | 1106.41 | Joback Method |

# Sources

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|---|---|
| **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 |
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=C52132613&Units=SI |

# Legend

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|---|---|
| **cpg:** | Ideal gas heat capacity |
| **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 |
| **tb:** | Normal Boiling Point Temperature |
| **tc:** | Critical Temperature |
| **tf:** | Normal melting (fusion) point |
| **vc:** | Critical Volume |