# 3-Nitro-4-methylbenzaldehyde

**Other names:** Benzaldehyde, 4-methyl-3-nitro-
4-Methyl-3-nitrobenzaldehyde
3-nitro-p-tolualdehyde
**Inchi:** InChI=1S/C8H7NO3/c1-6-2-3-7(5-10)4-8(6)9(11)12/h2-5H,1H3
**InchiKey:** KHWGAWBXQOKXIJ-UHFFFAOYSA-N
**Formula:** C8H7NO3
**SMILES:** Cc1ccc(C=O)cc1[N+](=O)[O-]
**Mol. weight [g/mol]:** 165.15
**CAS:** 31680-07-6

# Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | 45.66 | kJ/mol | Joback Method |
| hf | -91.20 | kJ/mol | Joback Method |
| hfus | 23.39 | kJ/mol | Joback Method |
| hvap | 60.31 | kJ/mol | Joback Method |
| log10ws | -2.84 | | Crippen Method |
| logp | 1.716 | | Crippen Method |
| mcvol | 118.810 | ml/mol | McGowan Method |
| pc | 3911.14 | kPa | Joback Method |
| tb | 619.58 | K | Joback Method |
| tc | 866.72 | K | Joback Method |
| tf | 416.99 | K | Joback Method |
| vc | 0.474 | m3/kmol | Joback Method |

# Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 276.16 | J/mol×K | 619.58 | Joback Method |
| cpg | 286.40 | J/mol×K | 660.77 | Joback Method |
| cpg | 295.87 | J/mol×K | 701.96 | Joback Method |
| cpg | 304.60 | J/mol×K | 743.15 | Joback Method |
| cpg | 312.63 | J/mol×K | 784.34 | Joback Method |
| cpg | 319.99 | J/mol×K | 825.53 | Joback Method |

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|---|---|---|---|---|
| cpg | 326.71 | J/mol×K | 866.72 | Joback Method |

# Sources

| | |
|---|---|
| **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=C31680076&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 |