# 4-Nitroguaiacol

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|---|---|
| **Other names:** | Phenol, 2-methoxy-4-nitro-<br>Guaiacol, 4-nitro-<br>Phenol, o-methoxy-p-nitro-<br>2-Methoxy-4-nitrophenol<br>3-Nitro-6-hydroxyanisole<br>4-Hydroxy-3-methoxynitrobenzene<br>o-Methoxy-p-nitrophenol |
| **Inchi:** | InChI=1S/C7H7NO4/c1-12-7-4-5(8(10)11)2-3-6(7)9/h2-4,9H,1H3 |
| **InchiKey:** | IZLVFLOBTPURLP-UHFFFAOYSA-N |
| **Formula:** | C7H7NO4 |
| **SMILES:** | COc1cc([N+](=O)[O-])ccc1O |
| **Mol. weight [g/mol]:** | 169.13 |
| **CAS:** | 3251-56-7 |

# Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -113.23 | kJ/mol | Joback Method |
| hf | -283.04 | kJ/mol | Joback Method |
| hfus | 25.87 | kJ/mol | Joback Method |
| hsub | 99.40 ± 2.00 | kJ/mol | NIST Webbook |
| hvap | 66.13 | kJ/mol | Joback Method |
| log10ws | -1.79 | | Crippen Method |
| logp | 1.309 | | Crippen Method |
| mcvol | 114.890 | ml/mol | McGowan Method |
| pc | 4890.21 | kPa | Joback Method |
| tb | 646.10 | K | Joback Method |
| tc | 901.50 | K | Joback Method |
| tf | 485.15 | K | Joback Method |
| vc | 0.386 | m3/kmol | Joback Method |

# Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 283.54 | J/mol×K | 646.10 | Joback Method |

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|---|---|---|---|---|
| cpg | 292.99 | J/mol×K | 688.67 | Joback Method |
| cpg | 301.75 | J/mol×K | 731.23 | Joback Method |
| cpg | 309.89 | J/mol×K | 773.80 | Joback Method |
| cpg | 317.50 | J/mol×K | 816.36 | Joback Method |
| cpg | 324.65 | J/mol×K | 858.93 | Joback Method |
| cpg | 331.41 | J/mol×K | 901.50 | Joback Method |
| hfust | 21.69 | kJ/mol | 374.40 | NIST Webbook |

# Sources

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|---|---|
| **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=C3251567&Units=SI |
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |
| **Crippen Method:** | https://www.chemeo.com/doc/models/crippen_log10ws |

# 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 |
| **hfust:** | Enthalpy of fusion at a given temperature |
| **hsub:** | Enthalpy of sublimation 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 |