

# 2-Methyl-5-nitrophenol

|                             |   |
|-----------------------------|---|
| <b>Other names:</b>         | Phenol, 2-methyl-5-nitro-o-Cresol, 5-nitro-2-Hydroxy-4-nitrotoluene<br>5-Nitro-2-cresol<br>5-nitro-o-cresol |
| <b>Inchi:</b>               | InChI=1S/C7H7NO3/c1-5-2-3-6(8(10)11)4-7(5)9/h2-4,9H,1H3   |
| <b>InchiKey:</b>            | UMFDLIXUUJMPSI-UHFFFAOYSA-N   |
| <b>Formula:</b>             | C7H7NO3   |
| <b>SMILES:</b>              | <chem>Cc1ccc([N+](=O)[O-])cc1O</chem>   |
| <b>Mol. weight [g/mol]:</b> | 153.14  |
| <b>CAS:</b>                 | 5428-54-6   |

## Physical Properties

| Property code | Value   | Unit    | Source         |
|---------------|---------|---------|----------------|
| gf            | -8.23   | kJ/mol  | Joback Method  |
| hf            | -150.82 | kJ/mol  | Joback Method  |
| hfus          | 24.68   | kJ/mol  | Joback Method  |
| hvap          | 63.72   | kJ/mol  | Joback Method  |
| log10ws       | -2.15   |         | Crippen Method |
| logp          | 1.609   |         | Crippen Method |
| mcvol         | 109.020 | ml/mol  | McGowan Method |
| pc            | 5008.59 | kPa     | Joback Method  |
| rinpol        | 1619.00 |         | NIST Webbook   |
| rinpol        | 1592.00 |         | NIST Webbook   |
| rinpol        | 1592.00 |         | NIST Webbook   |
| tb            | 623.68  | K       | Joback Method  |
| tc            | 883.67  | K       | Joback Method  |
| tf            | 462.92  | K       | Joback Method  |
| vc            | 0.367   | m3/kmol | Joback Method  |

## Temperature Dependent Properties

| Property code | Value  | Unit    | Temperature [K] | Source        |
|---------------|--------|---------|-----------------|---------------|
| cpg           | 262.28 | J/molxK | 623.68          | Joback Method |

|     |        |         |        |               |
|-----|--------|---------|--------|---------------|
| cpg | 271.81 | J/mol×K | 667.01 | Joback Method |
| cpg | 280.56 | J/mol×K | 710.34 | Joback Method |
| cpg | 288.66 | J/mol×K | 753.67 | Joback Method |
| cpg | 296.21 | J/mol×K | 797.01 | Joback Method |
| cpg | 303.32 | J/mol×K | 840.34 | Joback Method |
| cpg | 310.10 | J/mol×K | 883.67 | Joback Method |

## Sources

|                        |   |
|------------------------|---|
| <b>Joback Method:</b>  | <a href="https://en.wikipedia.org/wiki/Joback_method">https://en.wikipedia.org/wiki/Joback_method</a>                                       |
| <b>McGowan Method:</b> | <a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>                       |
| <b>NIST Webbook:</b>   | <a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C5428546&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C5428546&amp;Units=SI</a> |
| <b>Crippen Method:</b> | <a href="http://pubs.acs.org/doi/abs/10.1021/ci990307l">http://pubs.acs.org/doi/abs/10.1021/ci990307l</a>                                   |
| <b>Crippen Method:</b> | <a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>                           |

## Legend

|                 |   |
|-----------------|---|
| <b>cpg:</b>     | Ideal gas heat capacity                         |
| <b>gf:</b>      | Standard Gibbs free energy of formation         |
| <b>hf:</b>      | Enthalpy of formation at standard conditions    |
| <b>hfus:</b>    | Enthalpy of fusion at standard conditions       |
| <b>hvap:</b>    | Enthalpy of vaporization at standard conditions |
| <b>log10ws:</b> | Log10 of Water solubility in mol/l              |
| <b>logp:</b>    | Octanol/Water partition coefficient             |
| <b>mcvol:</b>   | McGowan's characteristic volume                 |
| <b>pc:</b>      | Critical Pressure                               |
| <b>rinpol:</b>  | Non-polar retention indices                     |
| <b>tb:</b>      | Normal Boiling Point Temperature                |
| <b>tc:</b>      | Critical Temperature                            |
| <b>tf:</b>      | Normal melting (fusion) point                   |
| <b>vc:</b>      | Critical Volume                                 |

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