# Phenol, 2-methyl-3,5-dinitro-

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|---|---|
| **Other names:** | o-Cresol, 3,5-dinitro- |
| | 3,5-Dinitro-o-cresol |
| | 4,6-Dinitro-2-hydroxytoluene |
| | 3,5-Dinitro-ortho-cresol |
| **Inchi:** | InChI=1S/C7H6N2O5/c1-4-6(9(13)14)2-5(8(11)12)3-7(4)10/h2-3,10H,1H3 |
| **InchiKey:** | KSHJAFFDLKPUMT-UHFFFAOYSA-N |
| **Formula:** | C7H6N2O5 |
| **SMILES:** | Cc1c(O)cc([N+](=O)[O-])cc1[N+](=O)[O-] |
| **Mol. weight [g/mol]:** | 198.13 |
| **CAS:** | 497-56-3 |

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | 17.69 | kJ/mol | Joback Method |
| hf | -173.05 | kJ/mol | Joback Method |
| hfus | 35.65 | kJ/mol | Joback Method |
| hvap | 80.97 | kJ/mol | Joback Method |
| log10ws | -2.80 | | Crippen Method |
| logp | 1.517 | | Crippen Method |
| mcvol | 126.440 | ml/mol | McGowan Method |
| pc | 4987.39 | kPa | Joback Method |
| tb | 780.50 | K | Joback Method |
| tc | 1059.76 | K | Joback Method |
| tf | 619.05 | K | Joback Method |
| vc | 0.450 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 334.95 | J/mol×K | 780.50 | Joback Method |
| cpg | 343.28 | J/mol×K | 827.04 | Joback Method |
| cpg | 351.09 | J/mol×K | 873.59 | Joback Method |
| cpg | 358.52 | J/mol×K | 920.13 | Joback Method |
| cpg | 365.69 | J/mol×K | 966.67 | Joback Method |

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|---|---|---|---|---|
| cpg | 372.74 | J/mol×K | 1013.21 | Joback Method |
| cpg | 379.80 | J/mol×K | 1059.76 | Joback Method |
| hsubt | 103.30 | kJ/mol | 307.00 | NIST Webbook |

# Sources

| | |
|---|---|
| **McGowan Method:** | http://link.springer.com/article/10.1007/BF02311772 |
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=C497563&Units=SI |
| **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 |

# 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 |
| **hsubt:** | Enthalpy of sublimation at a given temperature |
| **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 |