# Ethanone, 1-(2-nitrophenyl)-

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|---|---|
| **Other names:** | Acetophenone, 2'-nitro- |
| | o-Nitroacetophenone |
| | 2'-Nitroacetophenone |
| | 2-Nitroacetophenone |
| | 1-(2-Nitrophenyl)ethanone |
| | Methyl 2-nitrophenyl ketone |
| **Inchi:** | InChI=1S/C8H7NO3/c1-6(10)7-4-2-3-5-8(7)9(11)12/h2-5H,1H3 |
| **InchiKey:** | SUGXZLKUDLDTKX-UHFFFAOYSA-N |
| **Formula:** | C8H7NO3 |
| **SMILES:** | CC(=O)c1ccccc1[N+](=O)[O-] |
| **Mol. weight [g/mol]:** | 165.15 |
| **CAS:** | 577-59-3 |

# Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| ea | 1.40 ± 0.10 | eV | NIST Webbook |
| gf | 25.89 | kJ/mol | Joback Method |
| hf | -106.73 | kJ/mol | Joback Method |
| hfus | 23.09 | kJ/mol | Joback Method |
| hvap | 59.68 | kJ/mol | Joback Method |
| log10ws | -2.78 | | Crippen Method |
| logp | 1.797 | | Crippen Method |
| mcvol | 118.810 | ml/mol | McGowan Method |
| pc | 3930.78 | kPa | Joback Method |
| rinpol | 1456.50 | | NIST Webbook |
| rinpol | 1361.30 | | NIST Webbook |
| tb | 619.81 | K | Joback Method |
| tc | 871.76 | K | Joback Method |
| tf | 412.40 | K | Joback Method |
| vc | 0.464 | m3/kmol | Joback Method |

# Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|

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|---|---|---|---|---|
| cpg | 276.23 | J/mol×K | 619.81 | Joback Method |
| cpg | 287.00 | J/mol×K | 661.80 | Joback Method |
| cpg | 296.90 | J/mol×K | 703.79 | Joback Method |
| cpg | 305.97 | J/mol×K | 745.79 | Joback Method |
| cpg | 314.27 | J/mol×K | 787.78 | Joback Method |
| cpg | 321.82 | J/mol×K | 829.77 | Joback Method |
| cpg | 328.68 | J/mol×K | 871.76 | Joback Method |
| hvapt | 103.60 | kJ/mol | 313.00 | NIST Webbook |

# Pressure Dependent Properties

| Property code | Value | Unit | Pressure [kPa] | Source |
|---|---|---|---|---|
| tbrp | 432.20 | K | 2.10 | NIST Webbook |

# Sources

**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=C577593&Units=SI
**Crippen Method:** http://pubs.acs.org/doi/abs/10.1021/ci990307l
**Crippen Method:** https://www.chemeo.com/doc/models/crippen_log10ws

# Legend

**cpg:** Ideal gas heat capacity
**ea:** Electron affinity
**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
**hvapt:** Enthalpy of vaporization at a given temperature
**log10ws:** Log10 of Water solubility in mol/l
**logp:** Octanol/Water partition coefficient
**mcvol:** McGowan's characteristic volume
**pc:** Critical Pressure

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|---|---|
| **rinpol:** | Non-polar retention indices |
| **tb:** | Normal Boiling Point Temperature |
| **tbrp:** | Boiling point at reduced pressure |
| **tc:** | Critical Temperature |
| **tf:** | Normal melting (fusion) point |
| **vc:** | Critical Volume |