# 2-METHYL-2-NITRO-PROPANE-1,3-DIOL

| | |
|---|---|
| **Other names:** | 2-Methyl-2-nitro-1,3-propanediol |
| | 1,3-Propanediol, 2-methyl-2-nitro- |
| | Nitroisobutylglycol |
| | NMPD |
| | 1,1-Dimethylol-1-nitroethane |
| | 2-Methyl-2-nitropropane-1,3-diol |
| | 2-Methyl-2-nitropropanediol |
| | NSC 5372 |
| **Inchi:** | InChI=1S/C4H9NO4/c1-4(2-6,3-7)5(8)9/h6-7H,2-3H2,1H3 |
| **InchiKey:** | LOTYADDQWWVBDJ-UHFFFAOYSA-N |
| **Formula:** | C4H9NO4 |
| **SMILES:** | CC(CO)(CO)[N+](=O)[O-] |
| **Mol. weight [g/mol]:** | 135.12 |

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| chs | -2280.30 ± 2.80 | kJ/mol | NIST Webbook |
| chs | -2294.20 | kJ/mol | NIST Webbook |
| chs | -2289.80 ± 2.30 | kJ/mol | NIST Webbook |
| hf | -414.45 | kJ/mol | Cheméo Relay (1.0) |
| hfs | -570.50 ± 2.30 | kJ/mol | NIST Webbook |
| hfs | -580.10 ± 2.80 | kJ/mol | NIST Webbook |
| hfs | -566.10 | kJ/mol | NIST Webbook |
| hfus | 18.24 | kJ/mol | Joback Method |
| hvap | 71.94 | kJ/mol | Cheméo Relay (1.0) |
| log10ws | -1.15 | | Cheméo Relay (1.0) |
| logp | -0.994 | | Crippen Method |
| mcvol | 96.380 | ml/mol | McGowan Method |
| tb | 525.39 | K | Cheméo Relay (1.0) |
| tf | 424.00 ± 4.00 | K | NIST Webbook |

## Temperature Dependent Properties

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

| | | | | |
|---|---|---|---|---|
| cpg | 252.59 | J/mol×K | 623.89 | Joback Method |
| cpg | 259.45 | J/mol×K | 656.19 | Joback Method |
| cpg | 265.86 | J/mol×K | 688.49 | Joback Method |
| cpg | 271.86 | J/mol×K | 720.79 | Joback Method |
| cpg | 277.47 | J/mol×K | 753.10 | Joback Method |
| cpg | 282.72 | J/mol×K | 785.40 | Joback Method |
| cpg | 287.65 | J/mol×K | 817.70 | Joback Method |
| hfust | 3.84 | kJ/mol | 424.00 | NIST Webbook |

# Sources

**Cheméo Relay (1.0, beta):**

**NIST Webbook:** http://webbook.nist.gov/cgi/cbook.cgi?ID=C77496&Units=SI

**Joback Method:** https://en.wikipedia.org/wiki/Joback_method

**McGowan Method:** http://link.springer.com/article/10.1007/BF02311772

**Crippen Method:** http://pubs.acs.org/doi/abs/10.1021/ci990307l

**Crippen Method:** https://www.chemeo.com/doc/models/crippen_log10ws

**Cheméo Relay (1.0):**

# Legend

**chs:** Standard solid enthalpy of combustion
**cpg:** Ideal gas heat capacity
**hf:** Enthalpy of formation at standard conditions
**hfs:** Solid phase enthalpy of formation at standard conditions
**hfus:** Enthalpy of fusion at standard conditions
**hfust:** Enthalpy of fusion 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
**tb:** Normal Boiling Point Temperature
**tf:** Normal melting (fusion) point

Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.