# Methanediol, dinitrate

**Inchi:** InChI=1S/CH2N2O6/c4-2(5)8-1-9-3(6)7/h1H2
**InchiKey:** MKQRTTJKPCAWRP-UHFFFAOYSA-N
**Formula:** CH2N2O6
**SMILES:** O=[N+]([O-])OCO[N+](=O)[O-]
**Mol. weight [g/mol]:** 138.04
**CAS:** 38483-28-2

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| chl | -575.70 | kJ/mol | NIST Webbook |
| gf | -181.36 | kJ/mol | Joback Method |
| hf | -349.93 | kJ/mol | Joback Method |
| hfl | 93.30 | kJ/mol | NIST Webbook |
| hfus | 23.44 | kJ/mol | Joback Method |
| hvap | 55.82 | kJ/mol | Joback Method |
| log10ws | -1.06 | | Crippen Method |
| logp | -0.640 | | Crippen Method |
| mcvol | 71.530 | ml/mol | McGowan Method |
| pc | 5704.58 | kPa | Joback Method |
| tb | 570.80 | K | Joback Method |
| tc | 816.09 | K | Joback Method |
| tf | 432.71 | K | Joback Method |
| vc | 0.291 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 160.02 | J/mol×K | 570.80 | Joback Method |
| cpg | 165.72 | J/mol×K | 611.68 | Joback Method |
| cpg | 171.10 | J/mol×K | 652.56 | Joback Method |
| cpg | 176.15 | J/mol×K | 693.45 | Joback Method |
| cpg | 180.84 | J/mol×K | 734.33 | Joback Method |
| cpg | 185.12 | J/mol×K | 775.21 | Joback Method |
| cpg | 188.99 | J/mol×K | 816.09 | Joback Method |

# Sources

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|---|---|
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=C38483282&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 |
| **McGowan Method:** | http://link.springer.com/article/10.1007/BF02311772 |

# Legend

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|---|---|
| **chl:** | Standard liquid enthalpy of combustion |
| **cpg:** | Ideal gas heat capacity |
| **gf:** | Standard Gibbs free energy of formation |
| **hf:** | Enthalpy of formation at standard conditions |
| **hfl:** | Liquid phase enthalpy of formation at standard conditions |
| **hfus:** | Enthalpy of fusion 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 |