# Benzenesulfonic acid, 2,4-dinitro-

**Other names:** 2,4-Dinitrobenzenesulfonic acid
Kyselina 2,4-dinitrobenzensulfonova
2,4-Dinitrobenzenesulphonic acid
**Inchi:** InChI=1S/C6H4N2O7S/c9-7(10)4-1-2-6(16(13,14)15)5(3-4)8(11)12/h1-3H,(H,13,14,15)
**InchiKey:** OVOJUAKDTOOXRF-UHFFFAOYSA-N
**Formula:** C6H4N2O7S
**SMILES:** O=[N+]([O-])c1ccc(S(=O)(=O)O)c([N+](=O)[O-])c1
**Mol. weight [g/mol]:** 248.17
**CAS:** 89-02-1

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -441.47 | kJ/mol | Joback Method |
| hf | -580.68 | kJ/mol | Joback Method |
| hfus | 42.75 | kJ/mol | Joback Method |
| hvap | 101.05 | kJ/mol | Joback Method |
| log10ws | -2.36 | | Crippen Method |
| logp | 0.750 | | Crippen Method |
| mcvol | 140.440 | ml/mol | McGowan Method |
| pc | 6696.65 | kPa | Joback Method |
| tb | 816.96 | K | Joback Method |
| tc | 1059.01 | K | Joback Method |
| tf | 595.44 | K | Joback Method |
| vc | 0.573 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 363.89 | J/mol×K | 816.96 | Joback Method |
| cpg | 369.97 | J/mol×K | 857.30 | Joback Method |
| cpg | 375.19 | J/mol×K | 897.64 | Joback Method |
| cpg | 379.56 | J/mol×K | 937.99 | Joback Method |
| cpg | 383.08 | J/mol×K | 978.33 | Joback Method |
| cpg | 385.77 | J/mol×K | 1018.67 | Joback Method |

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|---|---|---|---|---|
| cpg | 387.63 | J/mol×K | 1059.01 | Joback Method |

# Sources

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|---|---|
| **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 |
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=C89021&Units=SI |
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |

# Legend

| | |
|---|---|
| **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 |
| **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 |