# Benzene, 1-ethoxy-2,4-dinitro-

**Other names:** 2,4-Dinitrophenetole
2,4-Dinitrophenyl ethyl ether
1-Ethoxy-2,4-dinitrobenzene
Phenetole, 2,4-dinitro-
2,4-Dinitro-1-ethoxy-benzene
2,4-Dinitrofenetol

**Inchi:** InChI=1S/C8H8N2O5/c1-2-15-8-4-3-6(9(11)12)5-7(8)10(13)14/h3-5H,2H2,1H3

**InchiKey:** YSOKMOXAGMIZFZ-UHFFFAOYSA-N

**Formula:** C8H8N2O5

**SMILES:** CCOc1ccc([N+](=O)[O-])cc1[N+](=O)[O-]

**Mol. weight [g/mol]:** 212.16

**CAS:** 610-54-8

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| chs | -4064.10 ± 4.10 | kJ/mol | NIST Webbook |
| chs | -4065.90 ± 4.10 | kJ/mol | NIST Webbook |
| gf | 75.73 | kJ/mol | Joback Method |
| hf | -148.60 | kJ/mol | Joback Method |
| hfus | 33.65 | kJ/mol | Joback Method |
| hvap | 72.59 | kJ/mol | Joback Method |
| log10ws | -3.31 | | Crippen Method |
| logp | 1.902 | | Crippen Method |
| mcvol | 140.530 | ml/mol | McGowan Method |
| pc | 3551.53 | kPa | Joback Method |
| tb | 745.18 | K | Joback Method |
| tc | 1007.50 | K | Joback Method |
| tf | 540.83 | K | Joback Method |
| vc | 0.557 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 371.15 | J/mol×K | 745.18 | Joback Method |

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|---|---|---|---|---|
| cpg | 381.49 | J/mol×K | 788.90 | Joback Method |
| cpg | 390.88 | J/mol×K | 832.62 | Joback Method |
| cpg | 399.33 | J/mol×K | 876.34 | Joback Method |
| cpg | 406.88 | J/mol×K | 920.06 | Joback Method |
| cpg | 413.54 | J/mol×K | 963.78 | Joback Method |
| cpg | 419.35 | J/mol×K | 1007.50 | Joback Method |

# Sources

| | |
|---|---|
| **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=C610548&Units=SI |
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |

# Legend

| | |
|---|---|
| **chs:** | Standard solid enthalpy of combustion |
| **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 |