# 2,4-Dinitro-N-ethylaniline

**Other names:** Benzenamine, N-ethyl-2,4-dinitro-
N-ethyl-2,4-dinitroaniline
**Inchi:** InChI=1S/C8H9N3O4/c1-2-9-7-4-3-6(10(12)13)5-8(7)11(14)15/h3-5,9H,2H2,1H3
**InchiKey:** YYOUTZBUOQBAAE-UHFFFAOYSA-N
**Formula:** C8H9N3O4
**SMILES:** CCNc1ccc([N+](=O)[O-])cc1[N+](=O)[O-]
**Mol. weight [g/mol]:** 211.17
**CAS:** 3846-50-2

# Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | 270.12 | kJ/mol | Joback Method |
| hf | 37.09 | kJ/mol | Joback Method |
| hfus | 37.56 | kJ/mol | Joback Method |
| hvap | 76.62 | kJ/mol | Joback Method |
| log10ws | -3.20 | | Crippen Method |
| logp | 1.935 | | Crippen Method |
| mcvol | 144.640 | ml/mol | McGowan Method |
| pc | 3682.02 | kPa | Joback Method |
| tb | 772.93 | K | Joback Method |
| tc | 1035.37 | K | Joback Method |
| tf | 571.26 | K | Joback Method |
| vc | 0.575 | m3/kmol | Joback Method |

# Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 393.67 | J/mol×K | 772.93 | Joback Method |
| cpg | 403.82 | J/mol×K | 816.67 | Joback Method |
| cpg | 413.03 | J/mol×K | 860.41 | Joback Method |
| cpg | 421.36 | J/mol×K | 904.15 | Joback Method |
| cpg | 428.86 | J/mol×K | 947.89 | Joback Method |
| cpg | 435.60 | J/mol×K | 991.63 | Joback Method |
| cpg | 441.61 | J/mol×K | 1035.37 | 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=C3846502&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 |