# 2-(4-Nitrophenoxy)ethanol

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|---|---|
| **Other names:** | 2-(p-Nitrophenoxy)ethanol |
| | Ethanol, 2-(4-nitrophenoxy)- |
| | «beta»-Hydroxyethyl p-nitrophenyl ether |
| | p-Nitrophenoxyethanol |
| | Ethanol, 2-(p-nitrophenoxy)- |
| **Inchi:** | InChI=1S/C8H9NO4/c10-5-6-13-8-3-1-7(2-4-8)9(11)12/h1-4,10H,5-6H2 |
| **InchiKey:** | YAPAEYFBLRVUMH-UHFFFAOYSA-N |
| **Formula:** | C8H9NO4 |
| **SMILES:** | O=[N+]([O-])c1ccc(OCCO)cc1 |
| **Mol. weight [g/mol]:** | 183.16 |
| **CAS:** | 16365-27-8 |

# Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -87.01 | kJ/mol | Joback Method |
| hf | -278.60 | kJ/mol | Joback Method |
| hfus | 26.77 | kJ/mol | Joback Method |
| hvap | 72.02 | kJ/mol | Joback Method |
| log10ws | -1.92 | | Crippen Method |
| logp | 0.966 | | Crippen Method |
| mcvol | 128.980 | ml/mol | McGowan Method |
| pc | 3990.60 | kPa | Joback Method |
| tb | 680.54 | K | Joback Method |
| tc | 901.43 | K | Joback Method |
| tf | 445.52 | K | Joback Method |
| vc | 0.494 | m3/kmol | Joback Method |

# Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 331.45 | J/mol×K | 680.54 | Joback Method |
| cpg | 341.05 | J/mol×K | 717.36 | Joback Method |
| cpg | 349.99 | J/mol×K | 754.17 | Joback Method |
| cpg | 358.27 | J/mol×K | 790.99 | Joback Method |

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|---|---|---|---|---|
| cpg | 365.93 | J/mol×K | 827.80 | Joback Method |
| cpg | 372.97 | J/mol×K | 864.62 | Joback Method |
| cpg | 379.42 | J/mol×K | 901.43 | Joback Method |

# Sources

| | |
|---|---|
| **McGowan Method:** | http://link.springer.com/article/10.1007/BF02311772 |
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=C16365278&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 |

# Legend

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