# Benzamide, 4-nitro-N-ethyl-N-hexyl-

**Inchi:** InChI=1S/C15H22N2O3/c1-3-5-6-7-12-16(4-2)15(18)13-8-10-14(11-9-13)17(19)20/h8-11
**InchiKey:** SPSZXGFYTQQXLX-UHFFFAOYSA-N
**Formula:** C15H22N2O3
**SMILES:** CCCCCCN(CC)C(=O)c1ccc([N+](=O)[O-])cc1
**Mol. weight [g/mol]:** 278.35

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | 195.61 | kJ/mol | Joback Method |
| hf | -183.68 | kJ/mol | Joback Method |
| hfus | 44.24 | kJ/mol | Joback Method |
| hvap | 77.30 | kJ/mol | Joback Method |
| log10ws | -4.78 | | Crippen Method |
| logp | 3.637 | | Crippen Method |
| mcvol | 227.420 | ml/mol | McGowan Method |
| pc | 1942.37 | kPa | Joback Method |
| rinpol | 2389.00 | | NIST Webbook |
| rinpol | 2389.00 | | NIST Webbook |
| tb | 792.41 | K | Joback Method |
| tc | 1010.62 | K | Joback Method |
| tf | 523.76 | K | Joback Method |
| vc | 0.874 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 673.48 | J/mol×K | 792.41 | Joback Method |
| cpg | 688.25 | J/mol×K | 828.78 | Joback Method |
| cpg | 701.98 | J/mol×K | 865.15 | Joback Method |
| cpg | 714.74 | J/mol×K | 901.52 | Joback Method |
| cpg | 726.59 | J/mol×K | 937.88 | Joback Method |
| cpg | 737.60 | J/mol×K | 974.25 | Joback Method |
| cpg | 747.81 | J/mol×K | 1010.62 | 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=U415291&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 |
| **rinpol:** | Non-polar retention indices |
| **tb:** | Normal Boiling Point Temperature |
| **tc:** | Critical Temperature |
| **tf:** | Normal melting (fusion) point |
| **vc:** | Critical Volume |