# 5-Acenaphthenamine, 4-nitro-

**Inchi:** InChI=1S/C12H10N2O2/c13-12-9-3-1-2-7-4-5-8(11(7)9)6-10(12)14(15)16/h1-3,6H,4-5,13
**InchiKey:** VWJYDQVCIUABSV-UHFFFAOYSA-N
**Formula:** C12H10N2O2
**SMILES:** Nc1c([N+](=O)[O-])cc2c3c(cccc13)CC2
**Mol. weight [g/mol]:** 214.22
**CAS:** 4657-95-8

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | 413.26 | kJ/mol | Joback Method |
| hf | 213.04 | kJ/mol | Joback Method |
| hfus | 32.06 | kJ/mol | Joback Method |
| hvap | 76.15 | kJ/mol | Joback Method |
| log10ws | -4.22 | | Crippen Method |
| logp | 2.429 | | Crippen Method |
| mcvol | 153.260 | ml/mol | McGowan Method |
| pc | 3686.49 | kPa | Joback Method |
| tb | 771.05 | K | Joback Method |
| tc | 1041.00 | K | Joback Method |
| tf | 586.77 | K | Joback Method |
| vc | 0.599 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 419.61 | J/mol×K | 771.05 | Joback Method |
| cpg | 430.65 | J/mol×K | 816.04 | Joback Method |
| cpg | 440.99 | J/mol×K | 861.03 | Joback Method |
| cpg | 450.82 | J/mol×K | 906.02 | Joback Method |
| cpg | 460.30 | J/mol×K | 951.01 | Joback Method |
| cpg | 469.62 | J/mol×K | 996.00 | Joback Method |
| cpg | 478.96 | J/mol×K | 1041.00 | Joback Method |

# Sources

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|---|---|
| **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 |
| **McGowan Method:** | http://link.springer.com/article/10.1007/BF02311772 |
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=C4657958&Units=SI |

# 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 |