# Nitrofen

**Other names:**
2',4'-Dichloro-4-nitrodiphenyl ether
2,4-Dichloro-4'-Nitrodiphenyl ether
2,4-Dichlorophenyl 4-nitrophenyl ether
2,4-Dichlorophenyl p-nitrophenyl ether
4'-Nitro-2,4-dichlorodiphenyl ether
4-(2,4-Dichlorophenoxy)nitrobenzene
4-Nitro-2',4'-dichlorophenyl ether
Benzene, 2,4-dichloro-1-(4-nitrophenoxy)-
Ether, 2,4-dichlorophenyl p-nitrophenyl
FW 925
Mezotox
NIP
Niclofen
Nitraphen
Nitrochlor
Nitrophen
Nitrophene
Preparation 125
TOK
TOK E
TOK E 25
TOK E 40
Trizilin
Trizilin 25

**Inchi:** InChI=1S/C12H7Cl2NO3/c13-8-1-6-12(11(14)7-8)18-10-4-2-9(3-5-10)15(16)17/h1-7H
**InchiKey:** XITQUSLLOSKDTB-UHFFFAOYSA-N
**Formula:** C12H7Cl2NO3
**SMILES:** O=[N+]([O-])c1ccc(Oc2ccc(Cl)cc2Cl)cc1
**Mol. weight [g/mol]:** 284.10
**CAS:** 1836-75-5

# Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | 152.78 | kJ/mol | Joback Method |
| hf | -26.82 | kJ/mol | Joback Method |
| hfus | 34.69 | kJ/mol | Joback Method |

| | | | |
|---|---|---|---|
| hvap | 76.61 | kJ/mol | Joback Method |
| log10ws | -5.46 | | Estimated Solubility Method |
| log10ws | -5.46 | | Aqueous Solubility Prediction Method |
| logp | 4.694 | | Crippen Method |
| mcvol | 180.190 | ml/mol | McGowan Method |
| pc | 2979.54 | kPa | Joback Method |
| rinpol | 2230.00 | | NIST Webbook |
| rinpol | 2173.00 | | NIST Webbook |
| rinpol | 2173.00 | | NIST Webbook |
| ripol | 3353.00 | | NIST Webbook |
| ripol | 3353.00 | | NIST Webbook |
| tb | 791.38 | K | Joback Method |
| tc | 1065.45 | K | Joback Method |
| tf | 343.32 | K | Aqueous Solubility Prediction Method |
| tf | 342.72 ± 0.20 | K | NIST Webbook |
| tf | 343.00 ± 1.00 | K | NIST Webbook |
| tf | 344.70 ± 0.20 | K | NIST Webbook |
| vc | 0.690 | m3/kmol | Joback Method |

# Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 469.92 | J/mol×K | 974.09 | Joback Method |
| cpg | 476.06 | J/mol×K | 1019.77 | Joback Method |
| cpg | 435.12 | J/mol×K | 791.38 | Joback Method |
| cpg | 445.46 | J/mol×K | 837.06 | Joback Method |
| cpg | 454.67 | J/mol×K | 882.74 | Joback Method |
| cpg | 462.81 | J/mol×K | 928.41 | Joback Method |
| cpg | 481.28 | J/mol×K | 1065.45 | Joback Method |
| hfust | 22.96 | kJ/mol | 342.00 | NIST Webbook |
| hfust | 2.70 | kJ/mol | 343.00 | NIST Webbook |
| hvapt | 115.90 | kJ/mol | 643.00 | NIST Webbook |
| hvapt | 90.40 | kJ/mol | 365.50 | NIST Webbook |
| sfust | 7.87 | J/mol×K | 343.00 | NIST Webbook |
| svapt | 180.20 | J/mol×K | 643.00 | NIST Webbook |

# Sources

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|---|---|
| **Joback Method:** | https://en.wikipedia.org/wiki/Joback_method |
| **Aqueous Solubility Prediction Method:** | http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa |
| **Estimated Solubility Method:** | http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt |
| **McGowan Method:** | http://link.springer.com/article/10.1007/BF02311772 |
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=C1836755&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 |
| **hfust:** | Enthalpy of fusion at a given temperature |
| **hvap:** | Enthalpy of vaporization at standard conditions |
| **hvapt:** | Enthalpy of vaporization at a given temperature |
| **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 |
| **ripol:** | Polar retention indices |
| **sfust:** | Entropy of fusion at a given temperature |
| **svapt:** | Entropy of vaporization at a given temperature |
| **tb:** | Normal Boiling Point Temperature |
| **tc:** | Critical Temperature |
| **tf:** | Normal melting (fusion) point |
| **vc:** | Critical Volume |