# Sulfanilanilide, 3-nitro-4-n-phenyl-

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|---|---|
| **Other names:** | 4-anilino-3-nitro-N-phenylbenzenesulphonamide |
| | Benzenesulfonamide, 3-nitro-N-phenyl-4-(phenylamino)- |
| **Inchi:** | InChI=1S/C18H15N3O4S/c22-21(23)18-13-16(26(24,25)20-15-9-5-2-6-10-15)11-12-17(1 |
| **InchiKey:** | BBFRYSKTTHYWQZ-UHFFFAOYSA-N |
| **Formula:** | C18H15N3O4S |
| **SMILES:** | O=[N+]([O-])c1cc(S(=O)(=O)Nc2ccccc2)ccc1Nc1ccccc1 |
| **Mol. weight [g/mol]:** | 369.39 |
| **CAS:** | 5124-25-4 |

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | 164.44 | kJ/mol | Joback Method |
| hf | -85.37 | kJ/mol | Joback Method |
| hfus | 56.66 | kJ/mol | Joback Method |
| hvap | 111.91 | kJ/mol | Joback Method |
| log10ws | -5.43 | | Crippen Method |
| logp | 4.139 | | Crippen Method |
| mcvol | 258.670 | ml/mol | McGowan Method |
| pc | 3121.00 | kPa | Joback Method |
| tb | 1001.20 | K | Joback Method |
| tc | 1266.03 | K | Joback Method |
| tf | 684.41 | K | Joback Method |
| vc | 0.998 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 775.81 | J/mol×K | 1001.20 | Joback Method |
| cpg | 784.51 | J/mol×K | 1045.34 | Joback Method |
| cpg | 791.75 | J/mol×K | 1089.48 | Joback Method |
| cpg | 797.64 | J/mol×K | 1133.61 | Joback Method |
| cpg | 802.29 | J/mol×K | 1177.75 | Joback Method |
| cpg | 805.79 | J/mol×K | 1221.89 | Joback Method |
| cpg | 808.26 | J/mol×K | 1266.03 | Joback Method |

# Sources

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|---|---|
| **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=C5124254&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 |

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