# Benzene, 1,4-diisocyanato-

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|---|---|
| **Other names:** | Isocyanic acid, p-phenylene ester |
| | p-Phenylene diisocyanate |
| | p-Phenylene isocyanate |
| | 1,4-Diisocyanatobenzene |
| | 1,4-Phenylene diisocyanate |
| | Phenylene-1,4-diisocyanate |
| | 1,4-Benzenediisocyanate |
| **Inchi:** | InChI=1S/C8H4N2O2/c11-5-9-7-1-2-8(4-3-7)10-6-12/h1-4H |
| **InchiKey:** | ALQLPWJFHRMHIU-UHFFFAOYSA-N |
| **Formula:** | C8H4N2O2 |
| **SMILES:** | O=C=Nc1ccc(N=C=O)cc1 |
| **Mol. weight [g/mol]:** | 160.13 |
| **CAS:** | 104-49-4 |

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| chs | -3696.00 | kJ/mol | NIST Webbook |
| hf | 5.79 | kJ/mol | Joback Method |
| hvap | 55.40 | kJ/mol | Joback Method |
| log10ws | -10.44 | | Crippen Method |
| logp | 1.621 | | Crippen Method |
| mcvol | 114.320 | ml/mol | McGowan Method |
| pc | 4316.89 | kPa | Joback Method |
| tb | 547.44 | K | Joback Method |
| tc | 777.94 | K | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cps | 211.70 | J/mol×K | 298.00 | NIST Webbook |

# Sources

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|---|---|
| **McGowan Method:** | http://link.springer.com/article/10.1007/BF02311772 |
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=C104494&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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|---|---|
| **chs:** | Standard solid enthalpy of combustion |
| **cps:** | Solid phase heat capacity |
| **hf:** | Enthalpy of formation 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 |