# 1-iodo-4-nitrobenzene

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| **Other names:** | 4-iodo-1-nitrobenzene |
| | 4-iodonitrobenzene |
| | 4-nitro-1-iodobenzene |
| | 4-nitroiodobenzene |
| | 4-nitrophenyl iodide |
| | benzene, 1-iodo-4-nitro- |
| | p-iodonitrobenzene |
| | p-nitroiodobenzene |
| | p-nitrophenyl iodide |
| **Inchi:** | InChI=1S/C6H4INO2/c7-5-1-3-6(4-2-5)8(9)10/h1-4H |
| **InchiKey:** | SCCCFNJTCDSLCY-UHFFFAOYSA-N |
| **Formula:** | C6H4INO2 |
| **SMILES:** | O=[N+]([O-])c1ccc(I)cc1 |
| **Mol. weight [g/mol]:** | 249.01 |

# Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | 196.09 | kJ/mol | Joback Method |
| hf | 124.00 | kJ/mol | Joback Method |
| hfus | 20.72 | kJ/mol | Joback Method |
| hvap | 57.85 | kJ/mol | Joback Method |
| log10ws | -3.27 | | Crippen Method |
| logp | 2.199 | | Crippen Method |
| mcvol | 114.880 | ml/mol | McGowan Method |
| pc | 4516.42 | kPa | Joback Method |
| tb | 613.32 | K | Joback Method |
| tc | 902.66 | K | Joback Method |
| tf | 397.99 | K | Joback Method |
| vc | 0.433 | m3/kmol | Joback Method |

# Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 214.25 | J/mol×K | 613.32 | Joback Method |

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| cpg | 222.78 | J/mol×K | 661.54 | Joback Method |
| cpg | 230.44 | J/mol×K | 709.77 | Joback Method |
| cpg | 237.31 | J/mol×K | 757.99 | Joback Method |
| cpg | 243.47 | J/mol×K | 806.21 | Joback Method |
| cpg | 249.00 | J/mol×K | 854.43 | Joback Method |
| cpg | 253.99 | J/mol×K | 902.66 | Joback Method |
| hvapt | 98.20 | kJ/mol | 298.15 | Experimental and computational study of the thermochemistry of the three iodonitrobenzene isomers |
| psub | 1.51e-04 | kPa | 315.11 | Experimental and computational study of the thermochemistry of the three iodonitrobenzene isomers |
| psub | 1.14e-04 | kPa | 313.17 | Experimental and computational study of the thermochemistry of the three iodonitrobenzene isomers |
| psub | 1.52e-04 | kPa | 315.11 | Experimental and computational study of the thermochemistry of the three iodonitrobenzene isomers |
| psub | 1.93e-04 | kPa | 317.18 | Experimental and computational study of the thermochemistry of the three iodonitrobenzene isomers |
| psub | 2.30e-04 | kPa | 319.13 | Experimental and computational study of the thermochemistry of the three iodonitrobenzene isomers |
| psub | 2.83e-04 | kPa | 321.10 | Experimental and computational study of the thermochemistry of the three iodonitrobenzene isomers |

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| psub | 3.59e-04 | kPa | 323.18 | Experimental and computational study of the thermochemistry of the three iodonitrobenzene isomers |
| psub | 4.55e-04 | kPa | 325.18 | Experimental and computational study of the thermochemistry of the three iodonitrobenzene isomers |
| psub | 5.52e-04 | kPa | 327.12 | Experimental and computational study of the thermochemistry of the three iodonitrobenzene isomers |
| psub | 8.57e-04 | kPa | 331.18 | Experimental and computational study of the thermochemistry of the three iodonitrobenzene isomers |
| psub | 1.04e-03 | kPa | 333.11 | Experimental and computational study of the thermochemistry of the three iodonitrobenzene isomers |
| psub | 9.40e-05 | kPa | 311.18 | Experimental and computational study of the thermochemistry of the three iodonitrobenzene isomers |
| psub | 1.21e-04 | kPa | 313.17 | Experimental and computational study of the thermochemistry of the three iodonitrobenzene isomers |
| psub | 9.70e-05 | kPa | 311.18 | Experimental and computational study of the thermochemistry of the three iodonitrobenzene isomers |
| psub | 1.79e-04 | kPa | 317.18 | Experimental and computational study of the thermochemistry of the three iodonitrobenzene isomers |

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| psub | 2.30e-04 | kPa | 319.13 | Experimental and computational study of the thermochemistry of the three iodonitrobenzene isomers | |
| psub | 2.82e-04 | kPa | 321.10 | Experimental and computational study of the thermochemistry of the three iodonitrobenzene isomers | |
| psub | 3.55e-04 | kPa | 323.18 | Experimental and computational study of the thermochemistry of the three iodonitrobenzene isomers | |
| psub | 4.51e-04 | kPa | 325.18 | Experimental and computational study of the thermochemistry of the three iodonitrobenzene isomers | |
| psub | 5.50e-04 | kPa | 327.12 | Experimental and computational study of the thermochemistry of the three iodonitrobenzene isomers | |
| psub | 6.72e-04 | kPa | 329.18 | Experimental and computational study of the thermochemistry of the three iodonitrobenzene isomers | |
| psub | 8.56e-04 | kPa | 331.18 | Experimental and computational study of the thermochemistry of the three iodonitrobenzene isomers | |
| psub | 1.04e-03 | kPa | 333.11 | Experimental and computational study of the thermochemistry of the three iodonitrobenzene isomers | |

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| psub | 9.30e-05 | kPa | 311.18 | Experimental and computational study of the thermochemistry of the three iodonitrobenzene isomers | |
| psub | 1.18e-04 | kPa | 313.17 | Experimental and computational study of the thermochemistry of the three iodonitrobenzene isomers | |
| psub | 1.50e-04 | kPa | 315.11 | Experimental and computational study of the thermochemistry of the three iodonitrobenzene isomers | |
| psub | 1.79e-04 | kPa | 317.18 | Experimental and computational study of the thermochemistry of the three iodonitrobenzene isomers | |
| psub | 2.26e-04 | kPa | 319.13 | Experimental and computational study of the thermochemistry of the three iodonitrobenzene isomers | |
| psub | 2.77e-04 | kPa | 321.10 | Experimental and computational study of the thermochemistry of the three iodonitrobenzene isomers | |
| psub | 3.54e-04 | kPa | 323.18 | Experimental and computational study of the thermochemistry of the three iodonitrobenzene isomers | |
| psub | 4.36e-04 | kPa | 325.18 | Experimental and computational study of the thermochemistry of the three iodonitrobenzene isomers | |
| psub | 5.46e-04 | kPa | 327.12 | Experimental and computational study of the thermochemistry of the three iodonitrobenzene isomers | |

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| psub | 6.73e-04 | kPa | 329.18 | Experimental and computational study of the thermochemistry of the three iodonitrobenzene isomers |
| psub | 8.30e-04 | kPa | 331.18 | Experimental and computational study of the thermochemistry of the three iodonitrobenzene isomers |
| psub | 1.02e-03 | kPa | 333.11 | Experimental and computational study of the thermochemistry of the three iodonitrobenzene isomers |

# Sources

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| **Joback Method:** | https://en.wikipedia.org/wiki/Joback_method |
| **McGowan Method:** | http://link.springer.com/article/10.1007/BF02311772 |
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |
| **Crippen Method:** | https://www.chemeo.com/doc/models/crippen_log10ws |
| **Experimental and computational study of the thermochemistry of the three iodonitrobenzene isomers:** | https://www.doi.org/10.1016/j.jct.2012.09.031 |

# 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 |
| **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 |
| **psub:** | Sublimation pressure |
| **tb:** | Normal Boiling Point Temperature |

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|---|---|
| **tc:** | Critical Temperature |
| **tf:** | Normal melting (fusion) point |
| **vc:** | Critical Volume |