# 1,2-DIBROMO-4-NITROBENZENE

**Inchi:** InChI=1S/C6H3Br2NO2/c7-5-2-1-4(9(10)11)3-6(5)8/h1-3H
**InchiKey:** DLLDRYLYVHKDKK-UHFFFAOYSA-N
**Formula:** C6H3Br2NO2
**SMILES:** O=[N+]([O-])c1ccc(Br)c(Br)c1
**Mol. weight [g/mol]:** 280.90

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| hf | 96.30 | kJ/mol | Cheméo Relay (1.0) |
| hfus | 26.49 | kJ/mol | Joback Method |
| hvap | 78.62 | kJ/mol | Cheméo Relay (1.0) |
| ie | 9.76 | eV | Cheméo Relay (1.0) |
| log10ws | -4.11 | | Cheméo Relay (1.0) |
| logp | 3.120 | | Crippen Method |
| mcvol | 124.060 | ml/mol | McGowan Method |
| tb | 567.29 | K | Cheméo Relay (1.0) |
| tf | 376.53 | K | Cheméo Relay (1.0) |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 229.96 | J/mol×K | 657.48 | Joback Method |
| cpg | 237.11 | J/mol×K | 704.89 | Joback Method |
| cpg | 243.55 | J/mol×K | 752.31 | Joback Method |
| cpg | 249.34 | J/mol×K | 799.72 | Joback Method |
| cpg | 254.59 | J/mol×K | 847.14 | Joback Method |
| cpg | 259.35 | J/mol×K | 894.55 | Joback Method |
| cpg | 263.72 | J/mol×K | 941.96 | Joback Method |

## Sources

| | |
|---|---|
| **Crippen Method:** | https://www.chemeo.com/doc/models/crippen_log10ws |
| **Cheméo Relay (1.0):** | |
| **Cheméo Relay (1.0, beta):** | |
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=C5411507&Units=SI |
| **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 |

# Legend

| | |
|---|---|
| **cpg:** | Ideal gas heat capacity |
| **hf:** | Enthalpy of formation at standard conditions |
| **hfus:** | Enthalpy of fusion at standard conditions |
| **hvap:** | Enthalpy of vaporization at standard conditions |
| **ie:** | Ionization energy |
| **log10ws:** | Log10 of Water solubility in mol/l |
| **logp:** | Octanol/Water partition coefficient |
| **mcvol:** | McGowan's characteristic volume |
| **tb:** | Normal Boiling Point Temperature |
| **tf:** | Normal melting (fusion) point |