# 2,6-Diiodo-p-benzoquinone

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|---|---|
| **Other names:** | 2,6-Diiodo-4-benzoquinone<br>2,6-Diiodoquinone<br>2,5-Cyclohexadiene-1,4-dione, 2,6-diiodo-<br>p-Benzoquinone, 2,6-diiodo-<br>Diiodoquinone |
| **Inchi:** | InChI=1S/C6H2I2O2/c7-4-1-3(9)2-5(8)6(4)10/h1-2H |
| **InchiKey:** | KANJSWOVFIVFDI-UHFFFAOYSA-N |
| **Formula:** | C6H2I2O2 |
| **SMILES:** | O=C1C=C(I)C(=O)C(I)=C1 |
| **Mol. weight [g/mol]:** | 359.89 |
| **CAS:** | 20389-01-9 |

# Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -56.48 | kJ/mol | Joback Method |
| hf | -121.55 | kJ/mol | Joback Method |
| hfus | 11.56 | kJ/mol | Joback Method |
| hvap | 58.84 | kJ/mol | Joback Method |
| log10ws | -3.38 | | Crippen Method |
| logp | 1.776 | | Crippen Method |
| mcvol | 130.720 | ml/mol | McGowan Method |
| pc | 4516.42 | kPa | Joback Method |
| tb | 691.10 | K | Joback Method |
| tc | 1013.28 | K | Joback Method |
| tf | 448.12 | K | Joback Method |
| vc | 0.468 | m3/kmol | Joback Method |

# Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 219.44 | J/mol×K | 691.10 | Joback Method |
| cpg | 228.02 | J/mol×K | 744.80 | Joback Method |
| cpg | 235.71 | J/mol×K | 798.49 | Joback Method |
| cpg | 242.43 | J/mol×K | 852.19 | Joback Method |

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|---|---|---|---|---|
| cpg | 248.09 | J/mol×K | 905.89 | Joback Method |
| cpg | 252.61 | J/mol×K | 959.58 | Joback Method |
| cpg | 255.91 | J/mol×K | 1013.28 | Joback Method |

# Sources

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|---|---|
| **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 |
| **McGowan Method:** | http://link.springer.com/article/10.1007/BF02311772 |
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=C20389019&Units=SI |

# 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 |
| **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 |