# Isophthalaldehyde

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|---|---|
| **Other names:** | m-Phthalaldehyde |
| | Isophthalic dicarboxaldehyde |
| | Isophthaldehyde |
| | 1,3-Benzenedicarboxaldehyde |
| | Isophtaldehydes |
| **Inchi:** | InChI=1S/C8H6O2/c9-5-7-2-1-3-8(4-7)6-10/h1-6H |
| **InchiKey:** | IZALUMVGBVKPJD-UHFFFAOYSA-N |
| **Formula:** | C8H6O2 |
| **SMILES:** | O=Cc1cccc(C=O)c1 |
| **Mol. weight [g/mol]:** | 134.13 |
| **CAS:** | 626-19-7 |

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| ea | 1.01 ± 0.09 | eV | NIST Webbook |
| ea | 0.97 ± 0.09 | eV | NIST Webbook |
| gf | -79.78 | kJ/mol | Joback Method |
| hf | -154.55 | kJ/mol | Joback Method |
| hfus | 14.71 | kJ/mol | Joback Method |
| hvap | 49.78 | kJ/mol | Joback Method |
| log10ws | -1.95 | | Crippen Method |
| logp | 1.312 | | Crippen Method |
| mcvol | 102.960 | ml/mol | McGowan Method |
| pc | 4316.89 | kPa | Joback Method |
| ripol | 2341.00 | | NIST Webbook |
| tb | 511.42 | K | Joback Method |
| tc | 733.14 | K | Joback Method |
| tf | 362.00 ± 2.00 | K | NIST Webbook |
| vc | 0.409 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 208.76 | J/mol×K | 511.42 | Joback Method |

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|---|---|---|---|---|
| cpg | 218.33 | J/mol×K | 548.37 | Joback Method |
| cpg | 227.27 | J/mol×K | 585.33 | Joback Method |
| cpg | 235.61 | J/mol×K | 622.28 | Joback Method |
| cpg | 243.38 | J/mol×K | 659.23 | Joback Method |
| cpg | 250.59 | J/mol×K | 696.19 | Joback Method |
| cpg | 257.27 | J/mol×K | 733.14 | Joback Method |
| dvisc | 0.0025093 | Pa×s | 302.86 | Joback Method |
| dvisc | 0.0015427 | Pa×s | 337.62 | Joback Method |
| dvisc | 0.0010385 | Pa×s | 372.38 | Joback Method |
| dvisc | 0.0007480 | Pa×s | 407.14 | Joback Method |
| dvisc | 0.0005673 | Pa×s | 441.90 | Joback Method |
| dvisc | 0.0004480 | Pa×s | 476.66 | Joback Method |
| dvisc | 0.0003653 | Pa×s | 511.42 | Joback Method |

# Sources

**NIST Webbook:** http://webbook.nist.gov/cgi/cbook.cgi?ID=C626197&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
**McGowan Method:** http://link.springer.com/article/10.1007/BF02311772

# Legend

**cpg:** Ideal gas heat capacity
**dvisc:** Dynamic viscosity
**ea:** Electron affinity
**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
**ripol:** Polar retention indices
**tb:** Normal Boiling Point Temperature
**tc:** Critical Temperature

**tf:** Normal melting (fusion) point

**vc:** Critical Volume