# 2,3,6-TRICHLOROBENZALDEHYDE

**Other names:** Benzaldehyde, 2,3,6-trichloro-
**Inchi:** InChI=1S/C7H3Cl3O/c8-5-1-2-6(9)7(10)4(5)3-11/h1-3H
**InchiKey:** AURSMWWOMOVHBM-UHFFFAOYSA-N
**Formula:** C7H3Cl3O
**SMILES:** O=Cc1c(Cl)ccc(Cl)c1Cl
**Mol. weight [g/mol]:** 209.46

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| hf | -138.67 | kJ/mol | Cheméo Relay (1.0) |
| hfus | 21.64 | kJ/mol | Joback Method |
| hvap | 68.12 | kJ/mol | Cheméo Relay (1.0) |
| ie | 9.44 | eV | Cheméo Relay (1.0) |
| log10ws | -3.40 | | Cheméo Relay (1.0) |
| logp | 3.459 | | Crippen Method |
| mcvol | 124.020 | ml/mol | McGowan Method |
| tb | 541.87 | K | Cheméo Relay (1.0) |
| tf | 328.48 | K | Cheméo Relay (1.0) |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 216.23 | J/mol×K | 562.13 | Joback Method |
| cpg | 250.83 | J/mol×K | 801.27 | Joback Method |
| cpg | 246.17 | J/mol×K | 761.42 | Joback Method |
| cpg | 241.09 | J/mol×K | 721.56 | Joback Method |
| cpg | 235.58 | J/mol×K | 681.70 | Joback Method |
| cpg | 229.61 | J/mol×K | 641.84 | Joback Method |
| cpg | 223.17 | J/mol×K | 601.99 | Joback Method |
| dvisc | 0.0006051 | Pa×s | 463.26 | Joback Method |
| dvisc | 0.0003352 | Pa×s | 562.13 | Joback Method |
| dvisc | 0.0003982 | Pa×s | 529.17 | Joback Method |
| dvisc | 0.0004841 | Pa×s | 496.22 | Joback Method |
| dvisc | 0.0015051 | Pa×s | 364.39 | Joback Method |

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|---|---|---|---|---|
| dvisc | 0.0007826 | Pa×s | 430.30 | Joback Method |
| dvisc | 0.0010563 | Pa×s | 397.35 | Joback Method |

# Sources

| | |
|---|---|
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |
| **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=C4659476&Units=SI |
| **Joback Method:** | https://en.wikipedia.org/wiki/Joback_method |
| **McGowan Method:** | http://link.springer.com/article/10.1007/BF02311772 |

# Legend

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|---|---|
| **cpg:** | Ideal gas heat capacity |
| **dvisc:** | Dynamic viscosity |
| **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 |