# Benzoic acid, 2,4,6-trichloro-

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|---|---|
| **Other names:** | 2,4,6-Trichlorobenzoic acid |
| **Inchi:** | InChI=1S/C7H3Cl3O2/c8-3-1-4(9)6(7(11)12)5(10)2-3/h1-2H,(H,11,12) |
| **InchiKey:** | RAFFVQBMVYYTQS-UHFFFAOYSA-N |
| **Formula:** | C7H3Cl3O2 |
| **SMILES:** | O=C(O)c1c(Cl)cc(Cl)cc1Cl |
| **Mol. weight [g/mol]:** | 225.46 |
| **CAS:** | 50-43-1 |

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -209.95 | kJ/mol | Joback Method |
| hf | -297.72 | kJ/mol | Joback Method |
| hfus | 25.04 | kJ/mol | Joback Method |
| hvap | 72.02 | kJ/mol | Joback Method |
| log10ws | -3.59 | | Crippen Method |
| logp | 3.345 | | Crippen Method |
| mcvol | 129.890 | ml/mol | McGowan Method |
| pc | 4109.14 | kPa | Joback Method |
| tb | 659.52 | K | Joback Method |
| tc | 883.58 | K | Joback Method |
| tf | 433.14 | K | Joback Method |
| vc | 0.491 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 247.03 | J/mol×K | 659.52 | Joback Method |
| cpg | 252.82 | J/mol×K | 696.86 | Joback Method |
| cpg | 258.18 | J/mol×K | 734.21 | Joback Method |
| cpg | 263.13 | J/mol×K | 771.55 | Joback Method |
| cpg | 267.68 | J/mol×K | 808.89 | Joback Method |
| cpg | 271.85 | J/mol×K | 846.23 | Joback Method |
| cpg | 275.65 | J/mol×K | 883.58 | Joback Method |
| dvisc | 0.0012269 | Pa×s | 433.14 | Joback Method |

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|---|---|---|---|---|
| dvisc | 0.0006628 | Pa×s | 470.87 | Joback Method |
| dvisc | 0.0003923 | Pa×s | 508.60 | Joback Method |
| dvisc | 0.0002496 | Pa×s | 546.33 | Joback Method |
| dvisc | 0.0001684 | Pa×s | 584.06 | Joback Method |
| dvisc | 0.0001192 | Pa×s | 621.79 | Joback Method |
| dvisc | 0.0000877 | Pa×s | 659.52 | 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=C50431&Units=SI |

# Legend

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

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