# 3-CHLORO-2-HYDROXYBENZOIC ACID

**Other names:** Benzoic acid, 3-chloro-2-hydroxy-
Salicylic acid, 3-chloro-
**Inchi:** InChI=1S/C7H5ClO3/c8-5-3-1-2-4(6(5)9)7(10)11/h1-3,9H,(H,10,11)
**InchiKey:** PPINMMULCRBDOS-UHFFFAOYSA-N
**Formula:** C7H5ClO3
**SMILES:** O=C(O)c1cccc(Cl)c1O
**Mol. weight [g/mol]:** 172.57

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| hf | -508.23 | kJ/mol | Cheméo Relay (1.0) |
| hfus | 23.21 | kJ/mol | Joback Method |
| hvap | 90.25 | kJ/mol | Cheméo Relay (1.0) |
| ie | 8.78 | eV | Cheméo Relay (1.0) |
| log10ws | -2.27 | | Cheméo Relay (1.0) |
| logp | 1.744 | | Crippen Method |
| mcvol | 111.280 | ml/mol | McGowan Method |
| rinpol | 1548.00 | | NIST Webbook |
| rinpol | 1548.00 | | NIST Webbook |
| tb | 525.16 | K | Cheméo Relay (1.0) |
| tc | 854.81 | K | Cheméo Relay (1.0) |
| tf | 430.72 | K | Cheméo Relay (1.0) |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 249.69 | J/mol×K | 655.32 | Joback Method |
| cpg | 256.05 | J/mol×K | 692.75 | Joback Method |
| cpg | 261.95 | J/mol×K | 730.18 | Joback Method |
| cpg | 267.47 | J/mol×K | 767.61 | Joback Method |
| cpg | 272.67 | J/mol×K | 805.04 | Joback Method |
| cpg | 277.63 | J/mol×K | 842.47 | Joback Method |
| cpg | 282.40 | J/mol×K | 879.90 | Joback Method |
| dvisc | 0.0004187 | Pa×s | 459.98 | Joback Method |

| | | | | |
|---|---|---|---|---|
| dvisc | 0.0001872 | Pa×s | 492.54 | Joback Method |
| dvisc | 0.0000925 | Pa×s | 525.09 | Joback Method |
| dvisc | 0.0000496 | Pa×s | 557.65 | Joback Method |
| dvisc | 0.0000285 | Pa×s | 590.21 | Joback Method |
| dvisc | 0.0000174 | Pa×s | 622.76 | Joback Method |
| dvisc | 0.0000111 | Pa×s | 655.32 | Joback Method |

# Sources

| | |
|---|---|
| **McGowan Method:** | http://link.springer.com/article/10.1007/BF02311772 |
| **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=C1829329&Units=SI |
| **Joback Method:** | https://en.wikipedia.org/wiki/Joback_method |

# Legend

| | |
|---|---|
| **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 |
| **rinpol:** | Non-polar retention indices |
| **tb:** | Normal Boiling Point Temperature |
| **tc:** | Critical Temperature |
| **tf:** | Normal melting (fusion) point |