# 2-Chlorobenzoic acid, pentyl ester

**Other names:** Benzoic acid, 2-chloro, pentyl ester
**Inchi:** InChI=1S/C12H15ClO2/c1-2-3-6-9-15-12(14)10-7-4-5-8-11(10)13/h4-5,7-8H,2-3,6,9H2,1
**InchiKey:** SUCIUJIXAHNYGX-UHFFFAOYSA-N
**Formula:** C12H15ClO2
**SMILES:** CCCCCOC(=O)c1ccccc1Cl
**Mol. weight [g/mol]:** 226.70
**CAS:** 70086-68-9

# Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -92.91 | kJ/mol | Joback Method |
| hf | -326.49 | kJ/mol | Joback Method |
| hfus | 27.47 | kJ/mol | Joback Method |
| hvap | 58.79 | kJ/mol | Joback Method |
| log10ws | -4.07 | | Crippen Method |
| logp | 3.687 | | Crippen Method |
| mcvol | 175.860 | ml/mol | McGowan Method |
| pc | 2391.19 | kPa | Joback Method |
| rinpol | 1630.00 | | NIST Webbook |
| rinpol | 1637.00 | | NIST Webbook |
| rinpol | 1627.00 | | NIST Webbook |
| rinpol | 1617.00 | | NIST Webbook |
| rinpol | 1611.00 | | NIST Webbook |
| rinpol | 1622.00 | | NIST Webbook |
| rinpol | 1630.00 | | NIST Webbook |
| rinpol | 1644.30 | | NIST Webbook |
| rinpol | 1644.30 | | NIST Webbook |
| rinpol | 1617.00 | | NIST Webbook |
| ripol | 2248.00 | | NIST Webbook |
| ripol | 2248.00 | | NIST Webbook |
| ripol | 2240.00 | | NIST Webbook |
| ripol | 2240.00 | | NIST Webbook |
| ripol | 2249.00 | | NIST Webbook |
| ripol | 2283.00 | | NIST Webbook |
| ripol | 2211.00 | | NIST Webbook |
| ripol | 2229.00 | | NIST Webbook |
| tb | 619.34 | K | Joback Method |

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|---|---|---|---|
| tc | 830.22 | K | Joback Method |
| tf | 366.02 | K | Joback Method |
| vc | 0.672 | m3/kmol | Joback Method |

# Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 421.33 | J/mol×K | 619.34 | Joback Method |
| cpg | 435.34 | J/mol×K | 654.49 | Joback Method |
| cpg | 448.54 | J/mol×K | 689.63 | Joback Method |
| cpg | 460.94 | J/mol×K | 724.78 | Joback Method |
| cpg | 472.56 | J/mol×K | 759.93 | Joback Method |
| cpg | 483.41 | J/mol×K | 795.07 | Joback Method |
| cpg | 493.53 | J/mol×K | 830.22 | Joback Method |
| dvisc | 0.0015544 | Pa×s | 366.02 | Joback Method |
| dvisc | 0.0008929 | Pa×s | 408.24 | Joback Method |
| dvisc | 0.0005690 | Pa×s | 450.46 | Joback Method |
| dvisc | 0.0003918 | Pa×s | 492.68 | Joback Method |
| dvisc | 0.0002861 | Pa×s | 534.90 | Joback Method |
| dvisc | 0.0002188 | Pa×s | 577.12 | Joback Method |
| dvisc | 0.0001735 | Pa×s | 619.34 | Joback Method |

# Sources

**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=C70086689&Units=SI
**Crippen Method:** http://pubs.acs.org/doi/abs/10.1021/ci990307l
**Crippen Method:** https://www.chemeo.com/doc/models/crippen_log10ws

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