# 4-Chlorobenzoic acid, benzyl ester

**Other names:** 4-Chlorobenzoic acid, benzyl ester
Benzyl 4-chlorobenzoate
**Inchi:** InChI=1S/C14H11ClO2/c15-13-8-6-12(7-9-13)14(16)17-10-11-4-2-1-3-5-11/h1-9H,10H2
**InchiKey:** VBIOKGVOQMIBHO-UHFFFAOYSA-N
**Formula:** C14H11ClO2
**SMILES:** O=C(OCc1ccccc1)c1ccc(Cl)cc1
**Mol. weight [g/mol]:** 246.69

# Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| af | 0.5844 | | Cheméo Relay (1.0) |
| hf | -185.33 | kJ/mol | Cheméo Relay (1.0) |
| hfus | 26.69 | kJ/mol | Joback Method |
| hvap | 89.51 | kJ/mol | Cheméo Relay (1.0) |
| ie | 8.88 | eV | Cheméo Relay (1.0) |
| log10ws | -4.54 | | Cheméo Relay (1.0) |
| logp | 3.697 | | Crippen Method |
| mcvol | 180.280 | ml/mol | McGowan Method |
| pc | 2752.67 | kPa | Joback Method |
| rinpol | 1903.00 | | NIST Webbook |
| rinpol | 1899.00 | | NIST Webbook |
| rinpol | 1899.00 | | NIST Webbook |
| rinpol | 1914.00 | | NIST Webbook |
| rinpol | 1928.00 | | NIST Webbook |
| rinpol | 1944.00 | | NIST Webbook |
| rinpol | 1892.00 | | NIST Webbook |
| rinpol | 1866.00 | | NIST Webbook |
| rinpol | 1899.00 | | NIST Webbook |
| rinpol | 1928.00 | | NIST Webbook |
| rinpol | 1892.00 | | NIST Webbook |
| rinpol | 1881.00 | | NIST Webbook |
| ripol | 2801.00 | | NIST Webbook |
| ripol | 2787.00 | | NIST Webbook |
| ripol | 2832.00 | | NIST Webbook |
| ripol | 2801.00 | | NIST Webbook |
| ripol | 2740.00 | | NIST Webbook |
| ripol | 2772.00 | | NIST Webbook |

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|---|---|---|---|
| ripol | 2772.00 | | NIST Webbook |
| tb | 606.34 | K | Cheméo Relay (1.0) |
| tc | 859.08 | K | Cheméo Relay (1.0) |
| tf | 306.26 | K | Cheméo Relay (1.0) |
| vc | 0.654 | m3/kmol | Cheméo Relay (1.0) |

# Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 439.76 | J/mol×K | 691.78 | Joback Method |
| cpg | 453.56 | J/mol×K | 732.82 | Joback Method |
| cpg | 466.19 | J/mol×K | 773.85 | Joback Method |
| cpg | 477.72 | J/mol×K | 814.89 | Joback Method |
| cpg | 488.18 | J/mol×K | 855.92 | Joback Method |
| cpg | 497.64 | J/mol×K | 896.96 | Joback Method |
| cpg | 506.14 | J/mol×K | 938.00 | Joback Method |
| dvisc | 0.0011566 | Pa×s | 414.98 | Joback Method |
| dvisc | 0.0006831 | Pa×s | 461.11 | Joback Method |
| dvisc | 0.0004441 | Pa×s | 507.25 | Joback Method |
| dvisc | 0.0003102 | Pa×s | 553.38 | Joback Method |
| dvisc | 0.0002289 | Pa×s | 599.51 | Joback Method |
| dvisc | 0.0001765 | Pa×s | 645.65 | Joback Method |
| dvisc | 0.0001408 | Pa×s | 691.78 | Joback Method |

# Sources

**NIST Webbook:** http://webbook.nist.gov/cgi/cbook.cgi?ID=C67483732&Units=SI
**Joback Method:** https://en.wikipedia.org/wiki/Joback_method
**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):**

# Legend

| | |
|---|---|
| **af:** | Acentric Factor |
| **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 |
| **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 |