# Prop-2-ynyl 3-chlorobenzoate

**Other names:** Benzoic acid, 3-chloro, 2-propynyl ester
**Inchi:** InChI=1S/C10H7ClO2/c1-2-6-13-10(12)8-4-3-5-9(11)7-8/h1,3-5,7H,6H2
**InchiKey:** LTRKIUGMBLDIDV-UHFFFAOYSA-N
**Formula:** C10H7ClO2
**SMILES:** C#CCOC(=O)c1cccc(Cl)c1
**Mol. weight [g/mol]:** 194.61

# Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | 113.32 | kJ/mol | Joback Method |
| hf | 6.69 | kJ/mol | Joback Method |
| hfus | 25.27 | kJ/mol | Joback Method |
| hvap | 54.19 | kJ/mol | Joback Method |
| log10ws | -3.03 | | Crippen Method |
| logp | 2.130 | | Crippen Method |
| mcvol | 139.080 | ml/mol | McGowan Method |
| pc | 3439.94 | kPa | Joback Method |
| rinpol | 1411.00 | | NIST Webbook |
| rinpol | 1449.00 | | NIST Webbook |
| rinpol | 1420.00 | | NIST Webbook |
| rinpol | 1411.00 | | NIST Webbook |
| rinpol | 1404.00 | | NIST Webbook |
| rinpol | 1401.00 | | NIST Webbook |
| rinpol | 1449.00 | | NIST Webbook |
| rinpol | 1404.00 | | NIST Webbook |
| rinpol | 1408.00 | | NIST Webbook |
| ripol | 2231.00 | | NIST Webbook |
| ripol | 2194.00 | | NIST Webbook |
| ripol | 2214.00 | | NIST Webbook |
| ripol | 2208.00 | | NIST Webbook |
| ripol | 2231.00 | | NIST Webbook |
| ripol | 2222.00 | | NIST Webbook |
| ripol | 2207.00 | | NIST Webbook |
| ripol | 2194.00 | | NIST Webbook |
| tb | 563.70 | K | Joback Method |
| tc | 797.93 | K | Joback Method |
| tf | 390.45 | K | Joback Method |

| | | | |
|---|---|---|---|
| vc | 0.522 | m3/kmol | Joback Method |

# Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 287.86 | J/mol×K | 563.70 | Joback Method |
| cpg | 298.70 | J/mol×K | 602.74 | Joback Method |
| cpg | 308.81 | J/mol×K | 641.78 | Joback Method |
| cpg | 318.22 | J/mol×K | 680.82 | Joback Method |
| cpg | 326.94 | J/mol×K | 719.86 | Joback Method |
| cpg | 335.00 | J/mol×K | 758.89 | Joback Method |
| cpg | 342.43 | J/mol×K | 797.93 | Joback Method |

# Sources

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|---|---|
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=U373549&Units=SI |
| **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 |

# Legend

| | |
|---|---|
| **cpg:** | Ideal gas heat capacity |
| **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 |

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