# Benzoic acid, 2-chloro, (E)-2-butenyl ester

**Inchi:** InChI=1S/C11H11ClO2/c1-2-3-8-14-11(13)9-6-4-5-7-10(9)12/h2-7H,8H2,1H3/b3-2+
**InchiKey:** DRMGWSBFVQFAEC-NSCUHMNNSA-N
**Formula:** C11H11ClO2
**SMILES:** CC=CCOC(=O)c1ccccc1Cl
**Mol. weight [g/mol]:** 210.66

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -21.11 | kJ/mol | Joback Method |
| hf | -188.63 | kJ/mol | Joback Method |
| hfus | 25.08 | kJ/mol | Joback Method |
| hvap | 56.52 | kJ/mol | Joback Method |
| log10ws | -3.51 | | Crippen Method |
| logp | 3.073 | | Crippen Method |
| mcvol | 157.470 | ml/mol | McGowan Method |
| pc | 2778.85 | kPa | Joback Method |
| rinpol | 1529.00 | | NIST Webbook |
| rinpol | 1536.00 | | NIST Webbook |
| rinpol | 1540.00 | | NIST Webbook |
| rinpol | 1533.00 | | NIST Webbook |
| rinpol | 1522.00 | | NIST Webbook |
| rinpol | 1522.00 | | NIST Webbook |
| ripol | 2212.00 | | NIST Webbook |
| ripol | 2231.00 | | NIST Webbook |
| ripol | 2266.00 | | NIST Webbook |
| ripol | 2232.00 | | NIST Webbook |
| ripol | 2244.00 | | NIST Webbook |
| ripol | 2212.00 | | NIST Webbook |
| ripol | 2254.00 | | NIST Webbook |
| tb | 600.62 | K | Joback Method |
| tc | 824.35 | K | Joback Method |
| tf | 349.67 | K | Joback Method |
| vc | 0.597 | m3/kmol | Joback Method |

# Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 352.29 | J/mol×K | 600.62 | Joback Method |
| cpg | 364.97 | J/mol×K | 637.91 | Joback Method |
| cpg | 376.83 | J/mol×K | 675.20 | Joback Method |
| cpg | 387.90 | J/mol×K | 712.49 | Joback Method |
| cpg | 398.21 | J/mol×K | 749.77 | Joback Method |
| cpg | 407.80 | J/mol×K | 787.06 | Joback Method |
| cpg | 416.70 | J/mol×K | 824.35 | Joback Method |
| dvisc | 0.0014831 | Pa×s | 349.67 | Joback Method |
| dvisc | 0.0008442 | Pa×s | 391.50 | Joback Method |
| dvisc | 0.0005358 | Pa×s | 433.32 | Joback Method |
| dvisc | 0.0003684 | Pa×s | 475.14 | Joback Method |
| dvisc | 0.0002691 | Pa×s | 516.97 | Joback Method |
| dvisc | 0.0002060 | Pa×s | 558.79 | Joback Method |
| dvisc | 0.0001637 | Pa×s | 600.62 | Joback Method |

# Sources

**McGowan Method:** http://link.springer.com/article/10.1007/BF02311772
**NIST Webbook:** http://webbook.nist.gov/cgi/cbook.cgi?ID=R31024&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

# 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

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|---|---|
| **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 |