# Phenyl chloroformate

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|---|---|
| **Other names:** | Carbonochloridic acid, phenyl ester |
| | Formic acid, chloro-, phenyl ester |
| | Chloroformic acid phenyl ester |
| | Phenoxycarbonyl chloride |
| | Phenyl chlorocarbonate |
| | Fenylester kyseliny chlormravenci |
| | UN 2746 |
| | NSC 210946 |
| **Inchi:** | InChI=1S/C7H5ClO2/c8-7(9)10-6-4-2-1-3-5-6/h1-5H |
| **InchiKey:** | AHWALFGBDFAJAI-UHFFFAOYSA-N |
| **Formula:** | C7H5ClO2 |
| **SMILES:** | O=C(Cl)Oc1ccccc1 |
| **Mol. weight [g/mol]:** | 156.57 |
| **CAS:** | 1885-14-9 |

# Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -125.38 | kJ/mol | Joback Method |
| hf | -211.82 | kJ/mol | Joback Method |
| hfus | 14.91 | kJ/mol | Joback Method |
| hvap | 46.99 | kJ/mol | Joback Method |
| log10ws | -2.50 | | Crippen Method |
| logp | 2.424 | | Crippen Method |
| mcvol | 105.410 | ml/mol | McGowan Method |
| pc | 4162.33 | kPa | Joback Method |
| tb | 499.96 | K | Joback Method |
| tc | 728.98 | K | Joback Method |
| tf | 297.15 | K | Joback Method |
| vc | 0.393 | m3/kmol | Joback Method |

# Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 196.73 | J/mol×K | 499.96 | Joback Method |

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|---|---|---|---|---|
| cpg | 206.29 | J/mol×K | 538.13 | Joback Method |
| cpg | 215.25 | J/mol×K | 576.30 | Joback Method |
| cpg | 223.60 | J/mol×K | 614.47 | Joback Method |
| cpg | 231.37 | J/mol×K | 652.64 | Joback Method |
| cpg | 238.57 | J/mol×K | 690.81 | Joback Method |
| cpg | 245.22 | J/mol×K | 728.98 | Joback Method |
| dvisc | 0.0022311 | Pa×s | 297.15 | Joback Method |
| dvisc | 0.0013130 | Pa×s | 330.95 | Joback Method |
| dvisc | 0.0008524 | Pa×s | 364.75 | Joback Method |
| dvisc | 0.0005955 | Pa×s | 398.56 | Joback Method |
| dvisc | 0.0004400 | Pa×s | 432.36 | Joback Method |
| dvisc | 0.0003397 | Pa×s | 466.16 | Joback Method |
| dvisc | 0.0002716 | Pa×s | 499.96 | Joback Method |

# Pressure Dependent Properties

| Property code | Value | Unit | Pressure [kPa] | Source |
|---|---|---|---|---|
| tbrp | 352.70 | K | 1.60 | NIST Webbook |

# Sources

**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
**NIST Webbook:** http://webbook.nist.gov/cgi/cbook.cgi?ID=C1885149&Units=SI

# 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

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|---|---|
| **log10ws:** | Log10 of Water solubility in mol/l |
| **logp:** | Octanol/Water partition coefficient |
| **mcvol:** | McGowan's characteristic volume |
| **pc:** | Critical Pressure |
| **tb:** | Normal Boiling Point Temperature |
| **tbrp:** | Boiling point at reduced pressure |
| **tc:** | Critical Temperature |
| **tf:** | Normal melting (fusion) point |
| **vc:** | Critical Volume |