# Benzoyl chloride, 4-methoxy-

| | |
|---|---|
| **Other names:** | p-Anisoyl chloride |
| | p-Methoxybenzoic acid chloride |
| | p-Methoxybenzoyl chloride |
| | Anisoyl chloride |
| | Benzoyl chloride, p-methoxy- |
| | 4-Methoxybenzoic acid chloride |
| | 4-Methoxybenzoyl chloride |
| | 4-Anisoyl chloride |
| | UN 1729 |
| | NSC 86125 |
| | Benzoyl chloride, methoxy- |
| | Methoxybenzoyl chloride |
| **Inchi:** | InChI=1S/C8H7ClO2/c1-11-7-4-2-6(3-5-7)8(9)10/h2-5H,1H3 |
| **InchiKey:** | MXMOTZIXVICDSD-UHFFFAOYSA-N |
| **Formula:** | C8H7ClO2 |
| **SMILES:** | COc1ccc(C(=O)Cl)cc1 |
| **Mol. weight [g/mol]:** | 170.59 |
| **CAS:** | 100-07-2 |

# Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -126.59 | kJ/mol | Joback Method |
| hf | -261.80 ± 5.10 | kJ/mol | NIST Webbook |
| hfl | -335.90 ± 2.90 | kJ/mol | NIST Webbook |
| hfus | 17.11 | kJ/mol | Joback Method |
| hvap | 74.10 ± 4.20 | kJ/mol | NIST Webbook |
| ie | 8.87 ± 0.05 | eV | NIST Webbook |
| log10ws | -2.48 | | Crippen Method |
| logp | 2.074 | | Crippen Method |
| mcvol | 119.500 | ml/mol | McGowan Method |
| pc | 3624.61 | kPa | Joback Method |
| rinpol | 1400.00 | | NIST Webbook |
| tb | 417.00 ± 3.00 | K | NIST Webbook |
| tc | 753.98 | K | Joback Method |
| tf | 294.00 ± 3.00 | K | NIST Webbook |
| vc | 0.449 | m3/kmol | Joback Method |

# Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 237.52 | J/mol×K | 527.82 | Joback Method |
| cpg | 247.94 | J/mol×K | 565.51 | Joback Method |
| cpg | 257.76 | J/mol×K | 603.21 | Joback Method |
| cpg | 266.97 | J/mol×K | 640.90 | Joback Method |
| cpg | 275.58 | J/mol×K | 678.59 | Joback Method |
| cpg | 283.61 | J/mol×K | 716.28 | Joback Method |
| cpg | 291.07 | J/mol×K | 753.98 | Joback Method |
| dvisc | 0.0017026 | Pa×s | 320.94 | Joback Method |
| dvisc | 0.0010543 | Pa×s | 355.42 | Joback Method |
| dvisc | 0.0007106 | Pa×s | 389.90 | Joback Method |
| dvisc | 0.0005107 | Pa×s | 424.38 | Joback Method |
| dvisc | 0.0003857 | Pa×s | 458.86 | Joback Method |
| dvisc | 0.0003030 | Pa×s | 493.34 | Joback Method |
| dvisc | 0.0002456 | Pa×s | 527.82 | Joback Method |

# Pressure Dependent Properties

| Property code | Value | Unit | Pressure [kPa] | Source |
|---|---|---|---|---|
| tbrp | 418.20 | K | 1.90 | NIST Webbook |

# 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=C100072&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 |
| **hfl:** | Liquid phase 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 |
| **tb:** | Normal Boiling Point Temperature |
| **tbrp:** | Boiling point at reduced pressure |
| **tc:** | Critical Temperature |
| **tf:** | Normal melting (fusion) point |
| **vc:** | Critical Volume |