# «alpha»,para-Dichloroanisole

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|---|---|
| **Other names:** | Benzene, 1-chloro-4-(chloromethoxy)-<br>«alpha»,4-Dichloroanisole |
| **Inchi:** | InChI=1S/C7H6Cl2O/c8-5-10-7-3-1-6(9)2-4-7/h1-4H,5H2 |
| **InchiKey:** | PJLGIZXAYTZSIZ-UHFFFAOYSA-N |
| **Formula:** | C7H6Cl2O |
| **SMILES:** | ClCOc1ccc(Cl)cc1 |
| **Mol. weight [g/mol]:** | 177.03 |
| **CAS:** | 21151-56-4 |

# Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -18.02 | kJ/mol | Joback Method |
| hf | -126.45 | kJ/mol | Joback Method |
| hfus | 17.12 | kJ/mol | Joback Method |
| hvap | 45.29 | kJ/mol | Joback Method |
| log10ws | -2.92 | | Crippen Method |
| logp | 2.915 | | Crippen Method |
| mcvol | 116.080 | ml/mol | McGowan Method |
| pc | 3607.21 | kPa | Joback Method |
| tb | 488.50 | K | Joback Method |
| tc | 714.16 | K | Joback Method |
| tf | 289.66 | K | Joback Method |
| vc | 0.435 | m3/kmol | Joback Method |

# Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 207.37 | J/mol×K | 488.50 | Joback Method |
| cpg | 249.73 | J/mol×K | 676.55 | Joback Method |
| cpg | 242.31 | J/mol×K | 638.94 | Joback Method |
| cpg | 234.38 | J/mol×K | 601.33 | Joback Method |
| cpg | 225.92 | J/mol×K | 563.72 | Joback Method |
| cpg | 216.92 | J/mol×K | 526.11 | Joback Method |
| cpg | 256.65 | J/mol×K | 714.16 | Joback Method |

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|---|---|---|---|---|
| dvisc | 0.0002428 | Pa×s | 488.50 | Joback Method |
| dvisc | 0.0002999 | Pa×s | 455.36 | Joback Method |
| dvisc | 0.0003828 | Pa×s | 422.22 | Joback Method |
| dvisc | 0.0005095 | Pa×s | 389.08 | Joback Method |
| dvisc | 0.0007150 | Pa×s | 355.94 | Joback Method |
| dvisc | 0.0010758 | Pa×s | 322.80 | Joback Method |
| dvisc | 0.0017773 | Pa×s | 289.66 | Joback Method |

# Pressure Dependent Properties

| Property code | Value | Unit | Pressure [kPa] | Source |
|---|---|---|---|---|
| tbrp | 395.20 | K | 2.40 | 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=C21151564&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
**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

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|---|---|
| **tc:** | Critical Temperature |
| **tf:** | Normal melting (fusion) point |
| **vc:** | Critical Volume |