

Benzenemethanol, 2-chloro-

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|-----------------------------|---|
| Other names: | Benzyl alcohol, o-chloro- o-Chlorobenzyl alcohol 2-Chlorobenzyl alcohol ortho-Chlorobenzyl alcohol (2-Chloro-phenyl)-methanol |
| Inchi: | InChI=1S/C7H7ClO/c8-7-4-2-1-3-6(7)5-9/h1-4,9H,5H2 |
| InchiKey: | MBYQPPXEXWRMQC-UHFFFAOYSA-N |
| Formula: | C7H7ClO |
| SMILES: | OCc1ccccc1Cl |
| Mol. weight [g/mol]: | 142.58 |
| CAS: | 17849-38-6 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|----------------------|----------------|
| gf | -37.91 | kJ/mol | Joback Method |
| hf | -130.72 | kJ/mol | Joback Method |
| hfus | 15.82 | kJ/mol | Joback Method |
| hvap | 55.18 | kJ/mol | Joback Method |
| log10ws | -2.30 | | Crippen Method |
| logp | 1.832 | | Crippen Method |
| mcpvol | 103.840 | ml/mol | McGowan Method |
| pc | 4333.96 | kPa | Joback Method |
| tb | 503.20 | K | NIST Webbook |
| tb | 500.20 | K | NIST Webbook |
| tc | 727.48 | K | Joback Method |
| tf | 298.33 | K | Joback Method |
| vc | 0.388 | m ³ /kmol | Joback Method |

Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---------------|--------|---------|-----------------|---------------|
| cpg | 204.63 | J/mol×K | 520.83 | Joback Method |
| cpg | 213.25 | J/mol×K | 555.27 | Joback Method |
| cpg | 221.36 | J/mol×K | 589.71 | Joback Method |

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|-------|-----------|---------|--------|---------------|
| cpg | 228.96 | J/molxK | 624.16 | Joback Method |
| cpg | 236.09 | J/molxK | 658.60 | Joback Method |
| cpg | 242.77 | J/molxK | 693.04 | Joback Method |
| cpg | 249.01 | J/molxK | 727.48 | Joback Method |
| dvisc | 0.0085009 | Paxs | 298.33 | Joback Method |
| dvisc | 0.0029645 | Paxs | 335.41 | Joback Method |
| dvisc | 0.0012750 | Paxs | 372.50 | Joback Method |
| dvisc | 0.0006389 | Paxs | 409.58 | Joback Method |
| dvisc | 0.0003591 | Paxs | 446.66 | Joback Method |
| dvisc | 0.0002205 | Paxs | 483.75 | Joback Method |
| dvisc | 0.0001451 | Paxs | 520.83 | Joback Method |

Pressure Dependent Properties

| Property code | Value | Unit | Pressure [kPa] | Source |
|---------------|--------|------|----------------|--------------|
| tbrp | 375.70 | K | 3.70 | NIST Webbook |

Sources

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|------------------------|---|
| 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=C17849386&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 |
| 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 |
| tc: | Critical Temperature |
| tf: | Normal melting (fusion) point |
| vc: | Critical Volume |

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<https://www.chemeo.com/cid/16-494-6/Benzenemethanol-2-chloro.pdf>

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