

Benzene, 1-chloro-3-(dichloromethyl)-

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| Other names: | 1-Chloro-3-(dichloromethyl)benzene |
| Inchi: | InChI=1S/C7H5Cl3/c8-6-3-1-2-5(4-6)7(9)10/h1-4,7H |
| InchiKey: | ACNQJGLSENYFQJ-UHFFFAOYSA-N |
| Formula: | C7H5Cl3 |
| SMILES: | Clc1cccc(C(Cl)Cl)c1 |
| Mol. weight [g/mol]: | 195.47 |
| CAS: | 15145-69-4 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|---------|----------------|
| gf | 72.61 | kJ/mol | Joback Method |
| hf | -15.25 | kJ/mol | Joback Method |
| hfus | 16.61 | kJ/mol | Joback Method |
| hvap | 46.88 | kJ/mol | Joback Method |
| log10ws | -3.80 | | Crippen Method |
| logp | 3.816 | | Crippen Method |
| mcvol | 122.450 | ml/mol | McGowan Method |
| pc | 3555.77 | kPa | Joback Method |
| rinpol | 1366.00 | | NIST Webbook |
| tb | 503.07 | K | Joback Method |
| tc | 742.51 | K | Joback Method |
| tf | 282.35 | K | Joback Method |
| vc | 0.461 | m3/kmol | Joback Method |

Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---------------|--------|---------|-----------------|---------------|
| cpg | 209.02 | J/molxK | 503.07 | Joback Method |
| cpg | 218.39 | J/molxK | 542.98 | Joback Method |
| cpg | 227.05 | J/molxK | 582.88 | Joback Method |
| cpg | 235.03 | J/molxK | 622.79 | Joback Method |
| cpg | 242.38 | J/molxK | 662.70 | Joback Method |
| cpg | 249.12 | J/molxK | 702.60 | Joback Method |
| cpg | 255.31 | J/molxK | 742.51 | Joback Method |

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|-------|-----------|------|--------|---------------|
| dvisc | 0.0029071 | Paxs | 282.35 | Joback Method |
| dvisc | 0.0015736 | Paxs | 319.14 | Joback Method |
| dvisc | 0.0009670 | Paxs | 355.92 | Joback Method |
| dvisc | 0.0006510 | Paxs | 392.71 | Joback Method |
| dvisc | 0.0004690 | Paxs | 429.50 | Joback Method |
| dvisc | 0.0003558 | Paxs | 466.28 | Joback Method |
| dvisc | 0.0002811 | Paxs | 503.07 | Joback Method |

Sources

| | |
|------------------------|---|
| NIST Webbook: | http://webbook.nist.gov/cgi/cbook.cgi?ID=C15145694&Units=SI |
| Crippen Method: | http://pubs.acs.org/doi/abs/10.1021/ci9903071 |
| Crippen Method: | https://www.cheméo.com/doc/models/crippen_log10ws |
| Joback Method: | https://en.wikipedia.org/wiki/Joback_method |
| McGowan Method: | http://link.springer.com/article/10.1007/BF02311772 |

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 |
| rinpol: | Non-polar retention indices |
| tb: | Normal Boiling Point Temperature |
| tc: | Critical Temperature |
| tf: | Normal melting (fusion) point |
| vc: | Critical Volume |

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