

1,2-Cyclobutane dicarbonyl chloride, trans-

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| Inchi: | InChI=1S/C6H6Cl2O2/c7-5(9)3-1-2-4(3)6(8)10/h3-4H,1-2H2 |
| InchiKey: | UKHMRFDNOROHX-UHFFFAOYSA-N |
| Formula: | C6H6Cl2O2 |
| SMILES: | O=C(Cl)C1CCC1C(=O)Cl |
| Mol. weight [g/mol]: | 181.02 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|---------|----------------|
| gf | -241.12 | kJ/mol | Joback Method |
| hf | -377.51 | kJ/mol | Joback Method |
| hfus | 19.99 | kJ/mol | Joback Method |
| hvap | 50.99 | kJ/mol | Joback Method |
| log10ws | -1.60 | | Crippen Method |
| logp | 1.543 | | Crippen Method |
| mcvol | 112.160 | ml/mol | McGowan Method |
| pc | 3810.39 | kPa | Joback Method |
| tb | 525.62 | K | Joback Method |
| tc | 750.40 | K | Joback Method |
| tf | 327.26 | K | Joback Method |
| vc | 0.429 | m3/kmol | Joback Method |

Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---------------|-----------|---------|-----------------|---------------|
| cpg | 225.63 | J/molxK | 525.62 | Joback Method |
| cpg | 235.90 | J/molxK | 563.08 | Joback Method |
| cpg | 245.47 | J/molxK | 600.55 | Joback Method |
| cpg | 254.35 | J/molxK | 638.01 | Joback Method |
| cpg | 262.59 | J/molxK | 675.47 | Joback Method |
| cpg | 270.21 | J/molxK | 712.93 | Joback Method |
| cpg | 277.25 | J/molxK | 750.40 | Joback Method |
| dvisc | 0.0027947 | Paxs | 327.26 | Joback Method |
| dvisc | 0.0020187 | Paxs | 360.32 | Joback Method |
| dvisc | 0.0015401 | Paxs | 393.38 | Joback Method |

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|-------|-----------|------|--------|---------------|
| dvisc | 0.0012253 | Paxs | 426.44 | Joback Method |
| dvisc | 0.0010074 | Paxs | 459.50 | Joback Method |
| dvisc | 0.0008504 | Paxs | 492.56 | Joback Method |
| dvisc | 0.0007333 | Paxs | 525.62 | Joback Method |

Sources

| | |
|------------------------|---|
| McGowan Method: | http://link.springer.com/article/10.1007/BF02311772 |
| NIST Webbook: | http://webbook.nist.gov/cgi/cbook.cgi?ID=B6006697&Units=SI |
| Crippen Method: | http://pubs.acs.org/doi/abs/10.1021/ci9903071 |
| Crippen Method: | https://www.chemeo.com/doc/models/crippen_log10ws |
| Joback Method: | https://en.wikipedia.org/wiki/Joback_method |

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

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