

Benzene, (2,2-dichloro-1-methylcyclopropyl)-

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| Other names: | (2,2-Dichloro-1-methylcyclopropyl)benzene |
| Inchi: | InChI=1S/C10H10Cl2/c1-9(7-10(9,11)12)8-5-3-2-4-6-8/h2-6H,7H2,1H3 |
| InchiKey: | NXYPRVQXSWVEOB-UHFFFAOYSA-N |
| Formula: | C10H10Cl2 |
| SMILES: | CC1(c2ccccc2)CC1(Cl)Cl |
| Mol. weight [g/mol]: | 201.09 |
| CAS: | 3591-42-2 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|---------|----------------|
| gf | 163.93 | kJ/mol | Joback Method |
| hf | 38.26 | kJ/mol | Joback Method |
| hfus | 10.70 | kJ/mol | Joback Method |
| hvap | 46.20 | kJ/mol | Joback Method |
| log10ws | -3.59 | | Crippen Method |
| logp | 3.522 | | Crippen Method |
| mcvol | 141.620 | ml/mol | McGowan Method |
| pc | 3325.84 | kPa | Joback Method |
| tb | 532.29 | K | Joback Method |
| tc | 786.07 | K | Joback Method |
| tf | 350.22 | K | Joback Method |
| vc | 0.537 | m3/kmol | Joback Method |

Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---------------|--------|---------|-----------------|---------------|
| cpg | 298.45 | J/molxK | 532.29 | Joback Method |
| cpg | 312.50 | J/molxK | 574.59 | Joback Method |
| cpg | 325.07 | J/molxK | 616.88 | Joback Method |
| cpg | 336.55 | J/molxK | 659.18 | Joback Method |
| cpg | 347.29 | J/molxK | 701.48 | Joback Method |
| cpg | 357.68 | J/molxK | 743.77 | Joback Method |
| cpg | 368.09 | J/molxK | 786.07 | Joback Method |

Pressure Dependent Properties

| Property code | Value | Unit | Pressure [kPa] | Source |
|---------------|--------|------|----------------|--------------|
| tbrp | 349.20 | K | 0.10 | 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=C3591422&Units=SI |
| Crippen Method: | http://pubs.acs.org/doi/abs/10.1021/ci9903071 |
| Crippen Method: | https://www.chemeo.com/doc/models/crippen_log10ws |

Legend

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|-----------------|---|
| cpg: | Ideal gas heat capacity |
| 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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