

Pentane, 2-chloro-3-methyl

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|-----------------------------|---|
| Inchi: | InChI=1S/C6H13Cl/c1-4-5(2)6(3)7/h5-6H,4H2,1-3H3 |
| InchiKey: | JPFZKJQZKBEPGQ-UHFFFAOYSA-N |
| Formula: | C6H13Cl |
| SMILES: | CCC(C)C(C)Cl |
| Mol. weight [g/mol]: | 120.62 |
| CAS: | 24319-09-3 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|----------------------|----------------|
| gf | -17.17 | kJ/mol | Joback Method |
| hf | -193.47 | kJ/mol | Joback Method |
| hfus | 8.45 | kJ/mol | Joback Method |
| hvap | 32.56 | kJ/mol | Joback Method |
| log10ws | -2.36 | | Crippen Method |
| logp | 2.660 | | Crippen Method |
| mcvol | 107.640 | ml/mol | McGowan Method |
| pc | 3035.62 | kPa | Joback Method |
| rinpol | 787.00 | | NIST Webbook |
| rinpol | 787.00 | | NIST Webbook |
| tb | 373.23 | K | Joback Method |
| tc | 553.82 | K | Joback Method |
| tf | 157.30 | K | Joback Method |
| vc | 0.408 | m ³ /kmol | Joback Method |

Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---------------|--------|---------|-----------------|---------------|
| cpg | 185.75 | J/molxK | 373.23 | Joback Method |
| cpg | 196.81 | J/molxK | 403.33 | Joback Method |
| cpg | 207.42 | J/molxK | 433.43 | Joback Method |
| cpg | 217.60 | J/molxK | 463.52 | Joback Method |
| cpg | 227.35 | J/molxK | 493.62 | Joback Method |
| cpg | 236.69 | J/molxK | 523.72 | Joback Method |
| cpg | 245.63 | J/molxK | 553.82 | Joback Method |

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|-------|-----------|------|--------|---------------|
| dvisc | 0.0170744 | Paxs | 157.30 | Joback Method |
| dvisc | 0.0045226 | Paxs | 193.29 | Joback Method |
| dvisc | 0.0018178 | Paxs | 229.28 | Joback Method |
| dvisc | 0.0009357 | Paxs | 265.26 | Joback Method |
| dvisc | 0.0005644 | Paxs | 301.25 | Joback Method |
| dvisc | 0.0003793 | Paxs | 337.24 | Joback Method |
| dvisc | 0.0002752 | Paxs | 373.23 | Joback Method |

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=C24319093&Units=SI |
| Crippen Method: | http://pubs.acs.org/doi/abs/10.1021/ci9903071 |
| Crippen Method: | https://www.cheméo.com/doc/models/crippen_log10ws |

Legend

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|-----------------|---|
| 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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