

ethanamine, 2-chloro, N-methyl, N-ethyl

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|----------------------|---|
| Inchi: | InChI=1S/C5H12ClN/c1-3-7(2)5-4-6/h3-5H2,1-2H3 |
| InchiKey: | LKFZXNUTEIHUEH-UHFFFAOYSA-N |
| Formula: | C5H12ClN |
| SMILES: | CCN(C)CCCl |
| Mol. weight [g/mol]: | 121.61 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|----------------------|----------------|
| gf | 90.07 | kJ/mol | Joback Method |
| hf | -94.74 | kJ/mol | Joback Method |
| hfus | 15.92 | kJ/mol | Joback Method |
| hvap | 33.15 | kJ/mol | Joback Method |
| log10ws | -0.64 | | Crippen Method |
| logp | 1.177 | | Crippen Method |
| mcvol | 103.530 | ml/mol | McGowan Method |
| pc | 3314.37 | kPa | Joback Method |
| rinpola | 837.72 | | NIST Webbook |
| rinpola | 837.72 | | NIST Webbook |
| tb | 363.67 | K | Joback Method |
| tc | 535.00 | K | Joback Method |
| tf | 208.50 | K | Joback Method |
| vc | 0.383 | m ³ /kmol | Joback Method |

Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---------------|--------|---------|-----------------|---------------|
| cpg | 176.35 | J/mol×K | 363.67 | Joback Method |
| cpg | 186.69 | J/mol×K | 392.22 | Joback Method |
| cpg | 196.59 | J/mol×K | 420.78 | Joback Method |
| cpg | 206.06 | J/mol×K | 449.33 | Joback Method |
| cpg | 215.11 | J/mol×K | 477.89 | Joback Method |
| cpg | 223.77 | J/mol×K | 506.44 | Joback Method |
| cpg | 232.04 | J/mol×K | 535.00 | Joback Method |

Sources

| | |
|------------------------|---|
| McGowan Method: | http://link.springer.com/article/10.1007/BF02311772 |
| NIST Webbook: | http://webbook.nist.gov/cgi/cbook.cgi?ID=R423499&Units=SI |
| Crippen Method: | http://pubs.acs.org/doi/abs/10.1021/ci990307l |
| Crippen Method: | https://www.cheméo.com/doc/models/crippen_log10ws |
| Joback Method: | https://en.wikipedia.org/wiki/Joback_method |

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 |
| h vap: | 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 |
| r in pol: | Non-polar retention indices |
| tb: | Normal Boiling Point Temperature |
| tc: | Critical Temperature |
| tf: | Normal melting (fusion) point |
| vc: | Critical Volume |

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