

Cyclopropanecarboxamide, N-(3-chlorophenyl)-

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|----------------------|--|
| Inchi: | InChI=1S/C10H10ClNO/c11-8-2-1-3-9(6-8)12-10(13)7-4-5-7/h1-3,6-7H,4-5H2,(H,12,13) |
| InchiKey: | QOGAQGLPMQVRTR-UHFFFAOYSA-N |
| Formula: | C10H10ClNO |
| SMILES: | O=C(Nc1cccc(Cl)c1)C1CC1 |
| Mol. weight [g/mol]: | 195.65 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|----------------------|----------------|
| gf | 145.39 | kJ/mol | Joback Method |
| hf | -26.72 | kJ/mol | Joback Method |
| hfus | 24.34 | kJ/mol | Joback Method |
| hvap | 58.27 | kJ/mol | Joback Method |
| log10ws | -2.85 | | Crippen Method |
| logp | 2.688 | | Crippen Method |
| mcvol | 140.930 | ml/mol | McGowan Method |
| pc | 3488.88 | kPa | Joback Method |
| rinsol | 1782.00 | | NIST Webbook |
| tb | 608.07 | K | Joback Method |
| tc | 844.37 | K | Joback Method |
| tf | 391.85 | K | Joback Method |
| vc | 0.534 | m ³ /kmol | Joback Method |

Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---------------|--------|---------|-----------------|---------------|
| cpg | 333.95 | J/mol×K | 608.07 | Joback Method |
| cpg | 347.01 | J/mol×K | 647.45 | Joback Method |
| cpg | 359.04 | J/mol×K | 686.84 | Joback Method |
| cpg | 370.12 | J/mol×K | 726.22 | Joback Method |
| cpg | 380.34 | J/mol×K | 765.60 | Joback Method |
| cpg | 389.77 | J/mol×K | 804.99 | Joback Method |
| cpg | 398.49 | J/mol×K | 844.37 | Joback Method |

Sources

| | |
|------------------------|---|
| NIST Webbook: | http://webbook.nist.gov/cgi/cbook.cgi?ID=U307187&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 |
| McGowan Method: | http://link.springer.com/article/10.1007/BF02311772 |

Legend

| | |
|-----------------|---|
| 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 |
| mccvol: | 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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