# N-(3-Chlorophenyl)-2,2,3,3,3-pentafluoropropanar

**Other names:** Propanamide, N-(3-chlorophenyl)-2,2,3,3,3-pentafluoro-
**Inchi:** InChI=1S/C9H5ClF5NO/c10-5-2-1-3-6(4-5)16-7(17)8(11,12)9(13,14)15/h1-4H,(H,16,17)
**InchiKey:** LHXBLOCHDJHVNH-UHFFFAOYSA-N
**Formula:** C9H5ClF5NO
**SMILES:** O=C(Nc1cccc(Cl)c1)C(F)(F)C(F)(F)F
**Mol. weight [g/mol]:** 273.59
**CAS:** 106376-32-3

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -892.15 | kJ/mol | Joback Method |
| hf | -1076.93 | kJ/mol | Joback Method |
| hfus | 24.19 | kJ/mol | Joback Method |
| hvap | 49.46 | kJ/mol | Joback Method |
| log10ws | -3.75 | | Crippen Method |
| logp | 3.476 | | Crippen Method |
| mcvol | 146.550 | ml/mol | McGowan Method |
| pc | 2729.71 | kPa | Joback Method |
| rinpol | 1291.00 | | NIST Webbook |
| rinpol | 1300.00 | | NIST Webbook |
| rinpol | 1300.00 | | NIST Webbook |
| tb | 568.34 | K | Joback Method |
| tc | 766.35 | K | Joback Method |
| tf | 370.43 | K | Joback Method |
| vc | 0.590 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 351.44 | J/mol×K | 568.34 | Joback Method |
| cpg | 361.75 | J/mol×K | 601.34 | Joback Method |
| cpg | 371.19 | J/mol×K | 634.34 | Joback Method |
| cpg | 379.81 | J/mol×K | 667.34 | Joback Method |
| cpg | 387.67 | J/mol×K | 700.35 | Joback Method |

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|---|---|---|---|---|
| cpg | 394.84 | J/mol×K | 733.35 | Joback Method |
| cpg | 401.36 | J/mol×K | 766.35 | Joback Method |

# Sources

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|---|---|
| **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 |
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=C106376323&Units=SI |
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |

# 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 |
| **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 |