# 1-Adamantanecarboxamide, N-(3-chlorophenyl)-

**Inchi:** InChI=1S/C17H20ClNO/c18-14-2-1-3-15(7-14)19-16(20)17-8-11-4-12(9-17)6-13(5-11)10

**InchiKey:** OWEPCGATVXVIDJ-UHFFFAOYSA-N

**Formula:** C17H20ClNO

**SMILES:** O=C(Nc1cccc(Cl)c1)C12CC3CC(CC(C3)C1)C2

**Mol. weight [g/mol]:** 289.80

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | 300.53 | kJ/mol | Joback Method |
| hf | -36.86 | kJ/mol | Joback Method |
| hfus | 31.41 | kJ/mol | Joback Method |
| hvap | 72.39 | kJ/mol | Joback Method |
| log10ws | -4.84 | | Crippen Method |
| logp | 4.495 | | Crippen Method |
| mcvol | 217.840 | ml/mol | McGowan Method |
| pc | 2338.29 | kPa | Joback Method |
| rinpol | 2532.00 | | NIST Webbook |
| rinpol | 2532.00 | | NIST Webbook |
| tb | 781.55 | K | Joback Method |
| tc | 1030.94 | K | Joback Method |
| tf | 522.76 | K | Joback Method |
| vc | 0.830 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 668.11 | J/mol×K | 781.55 | Joback Method |
| cpg | 686.93 | J/mol×K | 823.11 | Joback Method |
| cpg | 705.13 | J/mol×K | 864.68 | Joback Method |
| cpg | 723.04 | J/mol×K | 906.24 | Joback Method |
| cpg | 740.96 | J/mol×K | 947.81 | Joback Method |
| cpg | 759.21 | J/mol×K | 989.37 | Joback Method |
| cpg | 778.12 | J/mol×K | 1030.94 | Joback Method |

# Sources

| | |
|---|---|
| **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=U307467&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 |