# Propanamide, N-ethyl-N-(3-methylphenyl)-3-chloro-

**Inchi:** InChI=1S/C12H16ClNO/c1-3-14(12(15)7-8-13)11-6-4-5-10(2)9-11/h4-6,9H,3,7-8H2,1-2H
**InchiKey:** CBHNNONZIXWDRN-UHFFFAOYSA-N
**Formula:** C12H16ClNO
**SMILES:** CCN(C(=O)CCCl)c1cccc(C)c1
**Mol. weight [g/mol]:** 225.72

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | 122.87 | kJ/mol | Joback Method |
| hf | -126.74 | kJ/mol | Joback Method |
| hfus | 29.30 | kJ/mol | Joback Method |
| hvap | 58.42 | kJ/mol | Joback Method |
| log10ws | -3.04 | | Crippen Method |
| logp | 2.977 | | Crippen Method |
| mcvol | 179.970 | ml/mol | McGowan Method |
| pc | 2426.65 | kPa | Joback Method |
| rinpol | 1683.00 | | NIST Webbook |
| rinpol | 1683.00 | | NIST Webbook |
| tb | 609.36 | K | Joback Method |
| tc | 819.61 | K | Joback Method |
| tf | 376.26 | K | Joback Method |
| vc | 0.672 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 432.86 | J/mol×K | 609.36 | Joback Method |
| cpg | 447.62 | J/mol×K | 644.40 | Joback Method |
| cpg | 461.44 | J/mol×K | 679.44 | Joback Method |
| cpg | 474.38 | J/mol×K | 714.49 | Joback Method |
| cpg | 486.47 | J/mol×K | 749.53 | Joback Method |
| cpg | 497.76 | J/mol×K | 784.57 | Joback Method |
| cpg | 508.29 | J/mol×K | 819.61 | Joback Method |

# Sources

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|---|---|
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |
| **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=U308501&Units=SI |

# 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 |

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