# 2,2,3-Trichloro-n-(4-methylphenyl)propanamide

**Inchi:** InChI=1S/C10H10Cl3NO/c1-7-2-4-8(5-3-7)14-9(15)10(12,13)6-11/h2-5H,6H2,1H3,(H,14,
**InchiKey:** ZSTOEWMHZCPNGC-UHFFFAOYSA-N
**Formula:** C10H10Cl3NO
**SMILES:** Cc1ccc(NC(=O)C(Cl)(Cl)CCl)cc1
**Mol. weight [g/mol]:** 266.55
**CAS:** 28358-98-7

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | 63.62 | kJ/mol | Joback Method |
| hf | -139.75 | kJ/mol | Joback Method |
| hfus | 27.18 | kJ/mol | Joback Method |
| hvap | 65.83 | kJ/mol | Joback Method |
| log10ws | -3.64 | | Crippen Method |
| logp | 3.346 | | Crippen Method |
| mcvol | 176.270 | ml/mol | McGowan Method |
| pc | 2835.36 | kPa | Joback Method |
| tb | 672.96 | K | Joback Method |
| tc | 913.04 | K | Joback Method |
| tf | 436.17 | K | Joback Method |
| vc | 0.664 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 399.32 | J/mol×K | 672.96 | Joback Method |
| cpg | 410.32 | J/mol×K | 712.97 | Joback Method |
| cpg | 420.36 | J/mol×K | 752.99 | Joback Method |
| cpg | 429.52 | J/mol×K | 793.00 | Joback Method |
| cpg | 437.87 | J/mol×K | 833.01 | Joback Method |
| cpg | 445.51 | J/mol×K | 873.02 | Joback Method |
| cpg | 452.50 | J/mol×K | 913.04 | Joback Method |

# Sources

| | |
|---|---|
| **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=C28358987&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 |
| **tb:** | Normal Boiling Point Temperature |
| **tc:** | Critical Temperature |
| **tf:** | Normal melting (fusion) point |
| **vc:** | Critical Volume |