# 2,2,3-Trichloro-n-(4-chloro-2-methylphenyl)propan

**Inchi:** InChI=1S/C10H9Cl4NO/c1-6-4-7(12)2-3-8(6)15-9(16)10(13,14)5-11/h2-4H,5H2,1H3,(H,1
**InchiKey:** YVXKSFOYTJUMDP-UHFFFAOYSA-N
**Formula:** C10H9Cl4NO
**SMILES:** Cc1cc(Cl)ccc1NC(=O)C(Cl)(Cl)CCl
**Mol. weight [g/mol]:** 301.00
**CAS:** 116402-46-1

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | 42.06 | kJ/mol | Joback Method |
| hf | -166.96 | kJ/mol | Joback Method |
| hfus | 30.99 | kJ/mol | Joback Method |
| hvap | 70.88 | kJ/mol | Joback Method |
| log10ws | -4.32 | | Crippen Method |
| logp | 4.000 | | Crippen Method |
| mcvol | 188.510 | ml/mol | McGowan Method |
| pc | 2684.64 | kPa | Joback Method |
| tb | 715.37 | K | Joback Method |
| tc | 958.74 | K | Joback Method |
| tf | 478.61 | K | Joback Method |
| vc | 0.714 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 418.49 | J/mol×K | 715.37 | Joback Method |
| cpg | 428.20 | J/mol×K | 755.93 | Joback Method |
| cpg | 437.05 | J/mol×K | 796.49 | Joback Method |
| cpg | 445.11 | J/mol×K | 837.05 | Joback Method |
| cpg | 452.45 | J/mol×K | 877.62 | Joback Method |
| cpg | 459.17 | J/mol×K | 918.18 | Joback Method |
| cpg | 465.32 | J/mol×K | 958.74 | Joback Method |

# Sources

| | |
|---|---|
| **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=C116402461&Units=SI |
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |
| **Crippen Method:** | https://www.chemeo.com/doc/models/crippen_log10ws |

# Legend

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|---|---|
| **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 |