# 2,2,2'-Trichloro-n-butyl propionanilide

**Inchi:** InChI=1S/C13H16Cl3NO/c1-3-4-9-17(12(18)13(2,15)16)11-8-6-5-7-10(11)14/h5-8H,3-4,9
**InchiKey:** FRYHGFZDEVTUQV-UHFFFAOYSA-N
**Formula:** C13H16Cl3NO
**SMILES:** CCCCN(C(=O)C(C)(Cl)Cl)c1ccccc1Cl
**Mol. weight [g/mol]:** 308.63
**CAS:** 116402-44-9

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | 110.27 | kJ/mol | Joback Method |
| hf | -187.61 | kJ/mol | Joback Method |
| hfus | 32.87 | kJ/mol | Joback Method |
| hvap | 68.12 | kJ/mol | Joback Method |
| log10ws | -4.85 | | Crippen Method |
| logp | 4.667 | | Crippen Method |
| mcvol | 218.540 | ml/mol | McGowan Method |
| pc | 2102.27 | kPa | Joback Method |
| tb | 703.87 | K | Joback Method |
| tc | 928.95 | K | Joback Method |
| tf | 449.79 | K | Joback Method |
| vc | 0.816 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 539.16 | J/mol×K | 703.87 | Joback Method |
| cpg | 552.64 | J/mol×K | 741.38 | Joback Method |
| cpg | 565.08 | J/mol×K | 778.90 | Joback Method |
| cpg | 576.56 | J/mol×K | 816.41 | Joback Method |
| cpg | 587.16 | J/mol×K | 853.92 | Joback Method |
| cpg | 596.99 | J/mol×K | 891.43 | Joback Method |
| cpg | 606.11 | J/mol×K | 928.95 | 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=C116402449&Units=SI |
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |

# 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 |