# Propanamide, N,N-dibutyl-3-chloro-

**Inchi:** InChI=1S/C11H22ClNO/c1-3-5-9-13(10-6-4-2)11(14)7-8-12/h3-10H2,1-2H3
**InchiKey:** ALAPRJIGPQQKKY-UHFFFAOYSA-N
**Formula:** C11H22ClNO
**SMILES:** CCCCN(CCCC)C(=O)CCCl
**Mol. weight [g/mol]:** 219.75

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | 11.67 | kJ/mol | Joback Method |
| hf | -331.16 | kJ/mol | Joback Method |
| hfus | 33.06 | kJ/mol | Joback Method |
| hvap | 53.25 | kJ/mol | Joback Method |
| log10ws | -2.93 | | Crippen Method |
| logp | 3.044 | | Crippen Method |
| mcvol | 189.640 | ml/mol | McGowan Method |
| pc | 1975.31 | kPa | Joback Method |
| rinpol | 1592.00 | | NIST Webbook |
| rinpol | 1592.00 | | NIST Webbook |
| tb | 554.82 | K | Joback Method |
| tc | 729.73 | K | Joback Method |
| tf | 326.05 | K | Joback Method |
| vc | 0.725 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 456.11 | J/mol×K | 554.82 | Joback Method |
| cpg | 471.26 | J/mol×K | 583.97 | Joback Method |
| cpg | 485.71 | J/mol×K | 613.12 | Joback Method |
| cpg | 499.48 | J/mol×K | 642.28 | Joback Method |
| cpg | 512.60 | J/mol×K | 671.43 | Joback Method |
| cpg | 525.08 | J/mol×K | 700.58 | Joback Method |
| cpg | 536.95 | J/mol×K | 729.73 | 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=U308500&Units=SI |

# 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 |
| **rinpol:** | Non-polar retention indices |
| **tb:** | Normal Boiling Point Temperature |
| **tc:** | Critical Temperature |
| **tf:** | Normal melting (fusion) point |
| **vc:** | Critical Volume |