# Propionamide, 2,3-dichloro-N-3-methylbutyl-

**Inchi:** InChI=1S/C8H15Cl2NO/c1-6(2)3-4-11-8(12)7(10)5-9/h6-7H,3-5H2,1-2H3,(H,11,12)
**InchiKey:** KFBUGZALPNZPDM-UHFFFAOYSA-N
**Formula:** C8H15Cl2NO
**SMILES:** CC(C)CCNC(=O)C(Cl)CCl
**Mol. weight [g/mol]:** 212.12

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -51.79 | kJ/mol | Joback Method |
| hf | -309.60 | kJ/mol | Joback Method |
| hfus | 24.52 | kJ/mol | Joback Method |
| hvap | 54.58 | kJ/mol | Joback Method |
| log10ws | -2.31 | | Crippen Method |
| logp | 1.995 | | Crippen Method |
| mcvol | 159.610 | ml/mol | McGowan Method |
| pc | 2581.96 | kPa | Joback Method |
| rinpol | 1630.00 | | NIST Webbook |
| rinpol | 1630.00 | | NIST Webbook |
| tb | 560.46 | K | Joback Method |
| tc | 756.90 | K | Joback Method |
| tf | 312.35 | K | Joback Method |
| vc | 0.611 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 358.13 | J/mol×K | 560.46 | Joback Method |
| cpg | 370.44 | J/mol×K | 593.20 | Joback Method |
| cpg | 382.10 | J/mol×K | 625.94 | Joback Method |
| cpg | 393.13 | J/mol×K | 658.68 | Joback Method |
| cpg | 403.54 | J/mol×K | 691.42 | Joback Method |
| cpg | 413.36 | J/mol×K | 724.16 | Joback Method |
| cpg | 422.61 | J/mol×K | 756.90 | Joback Method |

# Sources

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|---|---|
| **McGowan Method:** | http://link.springer.com/article/10.1007/BF02311772 |
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=U415225&Units=SI |
| **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 |

# 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 |