# Z-3-Chloro-2-propyl-pent-2-enal

**Inchi:** InChI=1S/C9H15ClO/c1-3-5-8(7-11)9(10)6-4-2/h7H,3-6H2,1-2H3/b9-8-
**InchiKey:** LTPSZDYJWRDUSF-HJWRWDBZSA-N
**Formula:** C9H15ClO
**SMILES:** CCCC(Cl)=C(C=O)CCC
**Mol. weight [g/mol]:** 174.67

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -23.43 | kJ/mol | Joback Method |
| hf | -232.77 | kJ/mol | Joback Method |
| hfus | 23.13 | kJ/mol | Joback Method |
| hvap | 46.85 | kJ/mol | Joback Method |
| log10ws | -3.37 | | Crippen Method |
| logp | 3.278 | | Crippen Method |
| mcvol | 147.180 | ml/mol | McGowan Method |
| pc | 2543.05 | kPa | Joback Method |
| rinpol | 1019.90 | | NIST Webbook |
| ripol | 1412.20 | | NIST Webbook |
| tb | 495.33 | K | Joback Method |
| tc | 685.47 | K | Joback Method |
| tf | 230.11 | K | Joback Method |
| vc | 0.588 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 310.82 | J/mol×K | 495.33 | Joback Method |
| cpg | 323.50 | J/mol×K | 527.02 | Joback Method |
| cpg | 335.53 | J/mol×K | 558.71 | Joback Method |
| cpg | 346.94 | J/mol×K | 590.40 | Joback Method |
| cpg | 357.76 | J/mol×K | 622.09 | Joback Method |
| cpg | 368.01 | J/mol×K | 653.78 | Joback Method |
| cpg | 377.73 | J/mol×K | 685.47 | Joback Method |

# Sources

| | |
|---|---|
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=R154222&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 |
| **McGowan Method:** | http://link.springer.com/article/10.1007/BF02311772 |

# 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 |
| **ripol:** | Polar retention indices |
| **tb:** | Normal Boiling Point Temperature |
| **tc:** | Critical Temperature |
| **tf:** | Normal melting (fusion) point |
| **vc:** | Critical Volume |