# Propanamide, N,N-diundecyl-3-chloro-

**Inchi:** InChI=1S/C25H50ClNO/c1-3-5-7-9-11-13-15-17-19-23-27(25(28)21-22-26)24-20-18-16-1
**InchiKey:** ABKLQBLNOWQLPQ-UHFFFAOYSA-N
**Formula:** C25H50ClNO
**SMILES:** CCCCCCCCCCCN(CCCCCCCCCCC)C(=O)CCCl
**Mol. weight [g/mol]:** 416.12

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | 129.55 | kJ/mol | Joback Method |
| hf | -620.12 | kJ/mol | Joback Method |
| hfus | 69.32 | kJ/mol | Joback Method |
| hvap | 84.42 | kJ/mol | Joback Method |
| log10ws | -8.79 | | Crippen Method |
| logp | 8.506 | | Crippen Method |
| mcvol | 386.900 | ml/mol | McGowan Method |
| pc | 774.18 | kPa | Joback Method |
| rinpol | 3007.00 | | NIST Webbook |
| rinpol | 3007.00 | | NIST Webbook |
| tb | 875.14 | K | Joback Method |
| tc | 1072.37 | K | Joback Method |
| tf | 483.83 | K | Joback Method |
| vc | 1.508 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 1267.45 | J/mol×K | 875.14 | Joback Method |
| cpg | 1289.38 | J/mol×K | 908.01 | Joback Method |
| cpg | 1310.07 | J/mol×K | 940.88 | Joback Method |
| cpg | 1329.61 | J/mol×K | 973.75 | Joback Method |
| cpg | 1348.05 | J/mol×K | 1006.62 | Joback Method |
| cpg | 1365.48 | J/mol×K | 1039.50 | Joback Method |
| cpg | 1381.95 | J/mol×K | 1072.37 | 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=U308510&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 |