# Dichloroacetamide, N,N-dihexyl-

**Inchi:** InChI=1S/C14H27Cl2NO/c1-3-5-7-9-11-17(14(18)13(15)16)12-10-8-6-4-2/h13H,3-12H2,1
**InchiKey:** TXPVLEZUMVIIBX-UHFFFAOYSA-N
**Formula:** C14H27Cl2NO
**SMILES:** CCCCCCN(CCCCCC)C(=O)C(Cl)Cl
**Mol. weight [g/mol]:** 296.28

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | 22.56 | kJ/mol | Joback Method |
| hf | -414.10 | kJ/mol | Joback Method |
| hfus | 41.51 | kJ/mol | Joback Method |
| hvap | 63.93 | kJ/mol | Joback Method |
| log10ws | -4.94 | | Crippen Method |
| logp | 4.779 | | Crippen Method |
| mcvol | 244.150 | ml/mol | McGowan Method |
| pc | 1517.57 | kPa | Joback Method |
| rinpol | 1890.00 | | NIST Webbook |
| tb | 660.45 | K | Joback Method |
| tc | 839.33 | K | Joback Method |
| tf | 374.78 | K | Joback Method |
| vc | 0.935 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 644.09 | J/mol×K | 660.45 | Joback Method |
| cpg | 660.24 | J/mol×K | 690.26 | Joback Method |
| cpg | 675.58 | J/mol×K | 720.08 | Joback Method |
| cpg | 690.13 | J/mol×K | 749.89 | Joback Method |
| cpg | 703.94 | J/mol×K | 779.70 | Joback Method |
| cpg | 717.02 | J/mol×K | 809.52 | Joback Method |
| cpg | 729.41 | J/mol×K | 839.33 | Joback Method |

# Sources

| | |
|---|---|
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=U308634&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 |
| **tb:** | Normal Boiling Point Temperature |
| **tc:** | Critical Temperature |
| **tf:** | Normal melting (fusion) point |
| **vc:** | Critical Volume |