# Acetamide, 2,2,2-trichloro-

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|---|---|
| **Other names:** | «alpha»,«alpha»,«alpha»-Trichloroacetamide |
| | Trichloroacetamide |
| | 2,2,2-Trichloroacetamide |
| | Acetamide, «alpha»-trichloro- |
| | Amid kyseliny trichloroctove |
| | 2,2,2-Chloroacetamide |
| **Inchi:** | InChI=1S/C2H2Cl3NO/c3-2(4,5)1(6)7/h(H2,6,7) |
| **InchiKey:** | UPQQXPKAYZYUKO-UHFFFAOYSA-N |
| **Formula:** | C2H2Cl3NO |
| **SMILES:** | NC(=O)C(Cl)(Cl)Cl |
| **Mol. weight [g/mol]:** | 162.40 |
| **CAS:** | 594-65-0 |

# Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| chl | -3143.00 ± 33.00 | kJ/mol | NIST Webbook |
| chs | -779.10 | kJ/mol | NIST Webbook |
| gf | -129.46 | kJ/mol | Joback Method |
| hf | -219.37 | kJ/mol | Joback Method |
| hfus | 12.91 | kJ/mol | Joback Method |
| hvap | 49.29 | kJ/mol | Joback Method |
| ie | 10.53 | eV | NIST Webbook |
| log10ws | -1.43 | | Crippen Method |
| logp | 0.842 | | Crippen Method |
| mcvol | 87.310 | ml/mol | McGowan Method |
| pc | 5235.81 | kPa | Joback Method |
| tb | 512.20 | K | NIST Webbook |
| tc | 716.40 | K | Joback Method |
| tf | 337.67 | K | Joback Method |
| vc | 0.319 | m3/kmol | Joback Method |

# Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|

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|---|---|---|---|---|
| cpg | 142.26 | J/mol×K | 480.62 | Joback Method |
| cpg | 146.83 | J/mol×K | 519.92 | Joback Method |
| cpg | 150.88 | J/mol×K | 559.21 | Joback Method |
| cpg | 154.47 | J/mol×K | 598.51 | Joback Method |
| cpg | 157.62 | J/mol×K | 637.81 | Joback Method |
| cpg | 160.39 | J/mol×K | 677.10 | Joback Method |
| cpg | 162.82 | J/mol×K | 716.40 | Joback Method |

# Sources

| | |
|---|---|
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=C594650&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

| | |
|---|---|
| **chl:** | Standard liquid enthalpy of combustion |
| **chs:** | Standard solid enthalpy of combustion |
| **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 |
| **ie:** | Ionization energy |
| **log10ws:** | Log10 of Water solubility in mol/l |
| **logp:** | Octanol/Water partition coefficient |
| **mcvol:** | McGowan's characteristic volume |
| **pc:** | Critical Pressure |
| **tb:** | Normal Boiling Point Temperature |
| **tc:** | Critical Temperature |
| **tf:** | Normal melting (fusion) point |
| **vc:** | Critical Volume |

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