# 1(4H)-Pyridineacetic acid, 3,5-dichloro-4-oxo-

**Other names:** 3,5-dichloro-4-oxo-4H-pyridine-1-acetic acid
**Inchi:** InChI=1S/C7H5Cl2NO2/c8-4-1-3(7(11)12)2-5(9)6(4)10/h1-2H,10H2,(H,11,12)
**InchiKey:** UHXYYTSWBYTDPD-UHFFFAOYSA-N
**Formula:** C7H5Cl2NO3
**SMILES:** Nc1c(Cl)cc(C(=O)O)cc1Cl
**Mol. weight [g/mol]:** 222.03
**CAS:** 56187-37-2

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -131.57 | kJ/mol | Joback Method |
| hf | -248.19 | kJ/mol | Joback Method |
| hfus | 26.04 | kJ/mol | Joback Method |
| hvap | 78.27 | kJ/mol | Joback Method |
| log10ws | -2.54 | | Crippen Method |
| logp | 2.274 | | Crippen Method |
| mcvol | 127.630 | ml/mol | McGowan Method |
| pc | 4652.99 | kPa | Joback Method |
| tb | 694.62 | K | Joback Method |
| tc | 921.79 | K | Joback Method |
| tf | 486.48 | K | Joback Method |
| vc | 0.471 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 273.93 | J/mol×K | 694.62 | Joback Method |
| cpg | 280.35 | J/mol×K | 732.48 | Joback Method |
| cpg | 286.29 | J/mol×K | 770.34 | Joback Method |
| cpg | 291.76 | J/mol×K | 808.21 | Joback Method |
| cpg | 296.79 | J/mol×K | 846.07 | Joback Method |
| cpg | 301.40 | J/mol×K | 883.93 | Joback Method |
| cpg | 305.59 | J/mol×K | 921.79 | Joback Method |

# Sources

| | |
|---|---|
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=C56187372&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 |
| **tb:** | Normal Boiling Point Temperature |
| **tc:** | Critical Temperature |
| **tf:** | Normal melting (fusion) point |
| **vc:** | Critical Volume |