# 3,5-Dichlorophenoxyacetonitrile

**Inchi:** InChI=1S/C8H5Cl2NO/c9-6-3-7(10)5-8(4-6)12-2-1-11/h3-5H,2H2
**InchiKey:** PNROREDTZJCOHF-UHFFFAOYSA-N
**Formula:** C8H5Cl2NO
**SMILES:** N#CCOc1cc(Cl)cc(Cl)c1
**Mol. weight [g/mol]:** 202.04
**CAS:** 103140-12-1

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | 113.95 | kJ/mol | Joback Method |
| hf | 6.32 | kJ/mol | Joback Method |
| hfus | 20.83 | kJ/mol | Joback Method |
| hvap | 58.66 | kJ/mol | Joback Method |
| log10ws | -3.25 | | Crippen Method |
| logp | 2.896 | | Crippen Method |
| mcvol | 131.550 | ml/mol | McGowan Method |
| pc | 3082.99 | kPa | Joback Method |
| tb | 618.44 | K | Joback Method |
| tc | 857.15 | K | Joback Method |
| tf | 378.44 | K | Joback Method |
| vc | 0.517 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 262.20 | J/mol×K | 618.44 | Joback Method |
| cpg | 270.43 | J/mol×K | 658.22 | Joback Method |
| cpg | 278.10 | J/mol×K | 698.01 | Joback Method |
| cpg | 285.22 | J/mol×K | 737.79 | Joback Method |
| cpg | 291.81 | J/mol×K | 777.58 | Joback Method |
| cpg | 297.86 | J/mol×K | 817.36 | Joback Method |
| cpg | 303.39 | J/mol×K | 857.15 | Joback Method |

# Sources

| | |
|---|---|
| **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 |
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=C103140121&Units=SI |
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |

# Legend

| | |
|---|---|
| **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 |