# 4-Chloro-1,8-naphthalic anhydride

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| **Other names:** | 4-Chloronaphthalic anhydride |
| | 1H,3H-Naphtho[1,8-cd]pyran-1,3-dione, 6-chloro- |
| | 4-chloronaphthalene-1,8-dicarboxylic anhydride |
| **Inchi:** | InChI=1S/C12H5ClO3/c13-9-5-4-8-10-6(9)2-1-3-7(10)11(14)16-12(8)15/h1-5H |
| **InchiKey:** | UJEUBSWHCGDJQU-UHFFFAOYSA-N |
| **Formula:** | C12H5ClO3 |
| **SMILES:** | O=C1OC(=O)c2ccc(Cl)c3cccc1c23 |
| **Mol. weight [g/mol]:** | 232.62 |
| **CAS:** | 4053-08-1 |

# Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -34.44 | kJ/mol | Joback Method |
| hf | -227.82 | kJ/mol | Joback Method |
| hfus | 24.99 | kJ/mol | Joback Method |
| hvap | 65.82 | kJ/mol | Joback Method |
| log10ws | -4.42 | | Crippen Method |
| logp | 2.804 | | Crippen Method |
| mcvol | 147.110 | ml/mol | McGowan Method |
| pc | 3664.21 | kPa | Joback Method |
| tb | 745.99 | K | Joback Method |
| tc | 1020.48 | K | Joback Method |
| tf | 536.79 | K | Joback Method |
| vc | 0.564 | m3/kmol | Joback Method |

# Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 369.11 | J/mol×K | 745.99 | Joback Method |
| cpg | 380.25 | J/mol×K | 791.74 | Joback Method |
| cpg | 390.41 | J/mol×K | 837.49 | Joback Method |
| cpg | 399.63 | J/mol×K | 883.24 | Joback Method |
| cpg | 407.93 | J/mol×K | 928.99 | Joback Method |
| cpg | 415.37 | J/mol×K | 974.74 | Joback Method |

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|---|---|---|---|---|
| cpg | 421.98 | J/mol×K | 1020.48 | Joback Method |

# Sources

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|---|---|
| **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=C4053081&Units=SI |
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |

# 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 |