# Benzenesulfonyl chloride, 3,4-dichloro-

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| **Other names:** | 3,4-Dichlorobenzenesulfonyl chloride |
| | 3,4-Dichlorophenylsulfonyl chloride |
| | 3,4-dichlorobenzenesulphonyl chloride |
| **Inchi:** | InChI=1S/C6H3Cl3O2S/c7-5-2-1-4(3-6(5)8)12(9,10)11/h1-3H |
| **InchiKey:** | NYIBPWGZGSXURD-UHFFFAOYSA-N |
| **Formula:** | C6H3Cl3O2S |
| **SMILES:** | O=S(=O)(Cl)c1ccc(Cl)c(Cl)c1 |
| **Mol. weight [g/mol]:** | 245.51 |
| **CAS:** | 98-31-7 |

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -411.54 | kJ/mol | Joback Method |
| hf | -454.15 | kJ/mol | Joback Method |
| hfus | 28.53 | kJ/mol | Joback Method |
| hvap | 64.34 | kJ/mol | Joback Method |
| log10ws | -3.26 | | Crippen Method |
| logp | 2.921 | | Crippen Method |
| mcvol | 136.450 | ml/mol | McGowan Method |
| pc | 4762.81 | kPa | Joback Method |
| tb | 533.39 | K | Joback Method |
| tc | 762.90 | K | Joback Method |
| tf | 337.16 | K | Joback Method |
| vc | 0.536 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 237.72 | J/mol×K | 533.39 | Joback Method |
| cpg | 245.90 | J/mol×K | 571.64 | Joback Method |
| cpg | 253.51 | J/mol×K | 609.89 | Joback Method |
| cpg | 260.54 | J/mol×K | 648.15 | Joback Method |
| cpg | 267.00 | J/mol×K | 686.40 | Joback Method |
| cpg | 272.88 | J/mol×K | 724.65 | Joback Method |

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|---|---|---|---|---|
| cpg | 278.19 | J/mol×K | 762.90 | Joback Method |

# Sources

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|---|---|
| **McGowan Method:** | http://link.springer.com/article/10.1007/BF02311772 |
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=C98317&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 |

# 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 |