# 3-Chlorobenzenesulphonyl chloride

**Other names:** 3-chlorobenzenesulphonyl chloride
Benzenesulfonyl chloride, 3-chloro-
**Inchi:** InChI=1S/C6H4Cl2O2S/c7-5-2-1-3-6(4-5)11(8,9)10/h1-4H
**InchiKey:** OINWZUJVEXUHCC-UHFFFAOYSA-N
**Formula:** C6H4Cl2O2S
**SMILES:** O=S(=O)(Cl)c1cccc(Cl)c1
**Mol. weight [g/mol]:** 211.07

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| hf | -279.66 | kJ/mol | Cheméo Relay (1.0) |
| hfus | 24.72 | kJ/mol | Joback Method |
| hvap | 76.35 | kJ/mol | Cheméo Relay (1.0) |
| ie | 9.83 | eV | Cheméo Relay (1.0) |
| log10ws | -3.39 | | Cheméo Relay (1.0) |
| logp | 2.268 | | Crippen Method |
| mcvol | 124.210 | ml/mol | McGowan Method |
| tb | 537.21 | K | Cheméo Relay (1.0) |
| tf | 336.38 | K | Cheméo Relay (1.0) |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 217.31 | J/mol×K | 490.98 | Joback Method |
| cpg | 226.54 | J/mol×K | 528.18 | Joback Method |
| cpg | 235.17 | J/mol×K | 565.37 | Joback Method |
| cpg | 243.20 | J/mol×K | 602.57 | Joback Method |
| cpg | 250.65 | J/mol×K | 639.77 | Joback Method |
| cpg | 257.50 | J/mol×K | 676.96 | Joback Method |
| cpg | 263.77 | J/mol×K | 714.16 | Joback Method |

# Sources

| | |
|---|---|
| **McGowan Method:** | http://link.springer.com/article/10.1007/BF02311772 |
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |
| **Crippen Method:** | https://www.chemeo.com/doc/models/crippen_log10ws |
| **Cheméo Relay (1.0):** | |
| **Cheméo Relay (1.0, beta):** | |
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=C2888064&Units=SI |
| **Joback Method:** | https://en.wikipedia.org/wiki/Joback_method |

# Legend

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|---|---|
| **cpg:** | Ideal gas heat capacity |
| **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 |
| **tb:** | Normal Boiling Point Temperature |
| **tf:** | Normal melting (fusion) point |