# 4-Chlorophenylsulphonylacetone

**Other names:** 1-[(4-Chlorophenyl)sulfonyl]acetone
4-Chlorobenzenesulphonylpropan-2-one
4-Chlorophenylsulfonylpropan-2-one
Propan-2-one, 1-(4-chlorophenylsulphonyl)-
p-Chlorophenylsulfonylacetone
**Inchi:** InChI=1S/C9H9ClO3S/c1-7(11)6-14(12,13)9-4-2-8(10)3-5-9/h2-5H,6H2,1H3
**InchiKey:** BRDBHPZILGTBFY-UHFFFAOYSA-N
**Formula:** C9H9ClO3S
**SMILES:** CC(=O)CS(=O)(=O)c1ccc(Cl)cc1
**Mol. weight [g/mol]:** 232.69

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| hf | -443.19 | kJ/mol | Cheméo Relay (1.0) |
| hfus | 29.89 | kJ/mol | Joback Method |
| ie | 9.19 | eV | Cheméo Relay (1.0) |
| log10ws | -2.76 | | Cheméo Relay (1.0) |
| logp | 1.703 | | Crippen Method |
| mcvol | 155.810 | ml/mol | McGowan Method |
| tb | 602.06 | K | Cheméo Relay (1.0) |
| tf | 381.25 | K | Cheméo Relay (1.0) |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 335.62 | J/mol×K | 576.06 | Joback Method |
| cpg | 347.61 | J/mol×K | 612.05 | Joback Method |
| cpg | 358.80 | J/mol×K | 648.04 | Joback Method |
| cpg | 369.22 | J/mol×K | 684.03 | Joback Method |
| cpg | 378.87 | J/mol×K | 720.02 | Joback Method |
| cpg | 387.75 | J/mol×K | 756.01 | Joback Method |
| cpg | 395.88 | J/mol×K | 792.00 | Joback Method |

# Sources

| | |
|---|---|
| **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=C5000486&Units=SI |
| **Joback Method:** | https://en.wikipedia.org/wiki/Joback_method |
| **McGowan Method:** | http://link.springer.com/article/10.1007/BF02311772 |
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |

# Legend

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|---|---|
| **cpg:** | Ideal gas heat capacity |
| **hf:** | Enthalpy of formation at standard conditions |
| **hfus:** | Enthalpy of fusion 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 |