# 4-Chlorobenzenesulfonyl isocyanate

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|---|---|
| **Other names:** | p-Chlorobenzenesulfonyl isocyanate |
| **Inchi:** | InChI=1S/C7H4ClNO3S/c8-6-1-3-7(4-2-6)13(11,12)9-5-10/h1-4H |
| **InchiKey:** | JGHDVROWMPBQSR-UHFFFAOYSA-N |
| **Formula:** | C7H4ClNO3S |
| **SMILES:** | O=C=NS(=O)(=O)c1ccc(Cl)cc1 |
| **Mol. weight [g/mol]:** | 217.63 |
| **CAS:** | 5769-15-3 |

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| hf | -437.25 | kJ/mol | Joback Method |
| hvap | 66.67 | kJ/mol | Joback Method |
| log10ws | -6.34 | | Crippen Method |
| logp | 1.365 | | Crippen Method |
| mcvol | 133.310 | ml/mol | McGowan Method |
| pc | 5235.81 | kPa | Joback Method |
| tb | 543.10 | K | Joback Method |
| tc | 765.56 | K | Joback Method |

## Sources

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| **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 |
| **McGowan Method:** | http://link.springer.com/article/10.1007/BF02311772 |
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=C5769153&Units=SI |

## Legend

| | |
|---|---|
| **hf:** | Enthalpy of formation at standard conditions |
| **hvap:** | Enthalpy of vaporization at standard conditions |

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

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