# 2-Chloro-5-nitrophenyl isothiocyanate

**Other names:** 1-chloro-2-isothiocyanato-4-nitrobenzene
**Inchi:** InChI=1S/C7H3ClN2O2S/c8-6-2-1-5(10(11)12)3-7(6)9-4-13/h1-3H
**InchiKey:** QSSZYQDXSYYXKK-UHFFFAOYSA-N
**Formula:** C7H3ClN2O2S
**SMILES:** O=[N+]([O-])c1ccc(Cl)c(N=C=S)c1
**Mol. weight [g/mol]:** 214.63

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| hvap | 74.59 | kJ/mol | Cheméo Relay (1.0) |
| ie | 9.25 | eV | Cheméo Relay (1.0) |
| log10ws | -4.11 | | Cheméo Relay (1.0) |
| logp | 2.982 | | Crippen Method |
| mcvol | 133.120 | ml/mol | McGowan Method |
| tb | 537.43 | K | Cheméo Relay (1.0) |
| tf | 360.76 | K | Cheméo Relay (1.0) |

## Sources

**NIST Webbook:** http://webbook.nist.gov/cgi/cbook.cgi?ID=C57135689&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
**Crippen Method:** https://www.chemeo.com/doc/models/crippen_log10ws
**Cheméo Relay (1.0):**
**Cheméo Relay (1.0, beta):**

## Legend

**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 |