

# Chloromethyl thiocyanate

|                             |  |
|-----------------------------|--|
| <b>Other names:</b>         | Thiocyanic acid chloromethyl ester<br>Chloromethylthiocyanogen |
| <b>Inchi:</b>               | InChI=1S/C2H2CINS/c3-1-5-2-4/h1H2                              |
| <b>InchiKey:</b>            | UXUCVNXUWOLPRU-UHFFFAOYSA-N                                    |
| <b>Formula:</b>             | C2H2CINS   |
| <b>SMILES:</b>              | N#CSCCI  |
| <b>Mol. weight [g/mol]:</b> | 107.56   |
| <b>CAS:</b>                 | 3268-79-9  |

## Physical Properties

| Property code | Value   | Unit    | Source         |
|---------------|---------|---------|----------------|
| gf            | 120.33  | kJ/mol  | Joback Method  |
| hf            | 106.40  | kJ/mol  | Joback Method  |
| hfus          | 10.77   | kJ/mol  | Joback Method  |
| hvap          | 41.73   | kJ/mol  | Joback Method  |
| ie            | 10.29   | eV      | NIST Webbook   |
| log10ws       | -1.55   |         | Crippen Method |
| logp          | 1.397   |         | Crippen Method |
| mcvol         | 69.010  | ml/mol  | McGowan Method |
| pc            | 4723.61 | kPa     | Joback Method  |
| tb            | 458.20  | K       | NIST Webbook   |
| tc            | 683.47  | K       | Joback Method  |
| tf            | 241.61  | K       | Joback Method  |
| vc            | 0.277   | m3/kmol | Joback Method  |

## Temperature Dependent Properties

| Property code | Value  | Unit    | Temperature [K] | Source        |
|---------------|--------|---------|-----------------|---------------|
| cpg           | 101.24 | J/molxK | 453.45          | Joback Method |
| cpg           | 104.66 | J/molxK | 491.79          | Joback Method |
| cpg           | 107.92 | J/molxK | 530.12          | Joback Method |
| cpg           | 111.03 | J/molxK | 568.46          | Joback Method |
| cpg           | 113.98 | J/molxK | 606.79          | Joback Method |
| cpg           | 116.76 | J/molxK | 645.13          | Joback Method |

## Pressure Dependent Properties

| Property code | Value  | Unit | Pressure [kPa] | Source       |
|---------------|--------|------|----------------|--------------|
| tbrp          | 350.20 | K    | 2.00           | NIST Webbook |

## Sources

|                        |   |
|------------------------|---|
| <b>Crippen Method:</b> | <a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>                           |
| <b>Joback Method:</b>  | <a href="https://en.wikipedia.org/wiki/Joback_method">https://en.wikipedia.org/wiki/Joback_method</a>                                       |
| <b>McGowan Method:</b> | <a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>                       |
| <b>NIST Webbook:</b>   | <a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C3268799&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C3268799&amp;Units=SI</a> |
| <b>Crippen Method:</b> | <a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</a>                                   |

## Legend

|                 |   |
|-----------------|---|
| <b>cpg:</b>     | Ideal gas heat capacity                         |
| <b>gf:</b>      | Standard Gibbs free energy of formation         |
| <b>hf:</b>      | Enthalpy of formation at standard conditions    |
| <b>hfus:</b>    | Enthalpy of fusion at standard conditions       |
| <b>hvap:</b>    | Enthalpy of vaporization at standard conditions |
| <b>ie:</b>      | Ionization energy                               |
| <b>log10ws:</b> | Log10 of Water solubility in mol/l              |
| <b>logp:</b>    | Octanol/Water partition coefficient             |
| <b>mcvol:</b>   | McGowan's characteristic volume                 |
| <b>pc:</b>      | Critical Pressure                               |
| <b>tb:</b>      | Normal Boiling Point Temperature                |
| <b>tbrp:</b>    | Boiling point at reduced pressure               |
| <b>tc:</b>      | Critical Temperature                            |
| <b>tf:</b>      | Normal melting (fusion) point                   |
| <b>vc:</b>      | Critical Volume                                 |

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