

2-Chloroallyl isothiocyanate

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|-----------------------------|---|
| Other names: | 1-Propene, 2-chloro-3-isothiocyanato- |
| Inchi: | InChI=1S/C4H4CINS/c1-4(5)2-6-3-7/h1-2H2 |
| InchiKey: | DGBFPSVUFUDQNA-UHFFFAOYSA-N |
| Formula: | C4H4CINS |
| SMILES: | C=C(Cl)CN=C=S |
| Mol. weight [g/mol]: | 133.60 |
| CAS: | 14214-31-4 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|--------|----------------|
| hf | 258.08 | kJ/mol | Joback Method |
| hvap | 38.73 | kJ/mol | Joback Method |
| log10ws | -1.93 | | Crippen Method |
| logp | 1.842 | | Crippen Method |
| mcvol | 92.890 | ml/mol | McGowan Method |
| pc | 4056.96 | kPa | Joback Method |
| tb | 470.86 | K | Joback Method |
| tc | 708.46 | K | Joback Method |

Sources

| | |
|------------------------|---|
| McGowan Method: | http://link.springer.com/article/10.1007/BF02311772 |
| NIST Webbook: | http://webbook.nist.gov/cgi/cbook.cgi?ID=C14214314&Units=SI |
| Crippen Method: | http://pubs.acs.org/doi/abs/10.1021/ci990307I |
| Crippen Method: | https://www.chemeo.com/doc/models/crippen_log10ws |
| Joback Method: | https://en.wikipedia.org/wiki/Joback_method |

Legend

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

| | |
|-----------------|-------------------------------------|
| 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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