

2-Chlorophenyl isothiocyanate

Inchi: InChI=1S/C7H4CINS/c8-6-3-1-2-4-7(6)9-5-10/h1-4H
InchiKey: DASSPOJBUMBXLU-UHFFFAOYSA-N
Formula: C7H4CINS
SMILES: S=C=Nc1ccccc1Cl
Mol. weight [g/mol]: 169.63
CAS: 2740-81-0

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|--------|----------------|
| hf | 305.58 | kJ/mol | Joback Method |
| hvap | 48.94 | kJ/mol | Joback Method |
| log10ws | -3.07 | | Crippen Method |
| logp | 3.074 | | Crippen Method |
| mcvol | 115.700 | ml/mol | McGowan Method |
| pc | 3960.52 | kPa | Joback Method |
| tb | 574.60 | K | Joback Method |
| tc | 845.67 | K | Joback Method |

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C2740810&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
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>

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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