# 3-Pentane isothiocyanate

**Inchi:** InChI=1S/C6H11NS/c1-3-6(4-2)7-5-8/h6H,3-4H2,1-2H3
**InchiKey:** YDRYFNXKCXDLPP-UHFFFAOYSA-N
**Formula:** C6H11NS
**SMILES:** CCC(CC)N=C=S
**Mol. weight [g/mol]:** 129.22
**CAS:** 201224-89-7

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| hf | 111.62 | kJ/mol | Joback Method |
| hvap | 39.00 | kJ/mol | Joback Method |
| log10ws | -2.38 | | Crippen Method |
| logp | 2.278 | | Crippen Method |
| mcvol | 113.130 | ml/mol | McGowan Method |
| pc | 3213.68 | kPa | Joback Method |
| tb | 482.19 | K | Joback Method |
| tc | 701.74 | K | Joback Method |

## Sources

**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=C201224897&Units=SI
**Crippen Method:** http://pubs.acs.org/doi/abs/10.1021/ci990307l

## 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 |