# 2-Isopropylphenyl isothiocyanate

**Inchi:** InChI=1S/C10H11NS/c1-8(2)9-5-3-4-6-10(9)11-7-12/h3-6,8H,1-2H3
**InchiKey:** QQOOMDSEMQHMIR-UHFFFAOYSA-N
**Formula:** C10H11NS
**SMILES:** CC(C)c1ccccc1N=C=S
**Mol. weight [g/mol]:** 177.27
**CAS:** 36176-31-5

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| hf | 254.12 | kJ/mol | Joback Method |
| hvap | 50.84 | kJ/mol | Joback Method |
| log10ws | -3.57 | | Crippen Method |
| logp | 3.544 | | Crippen Method |
| mcvol | 145.730 | ml/mol | McGowan Method |
| pc | 2979.54 | kPa | Joback Method |
| tb | 605.37 | K | Joback Method |
| tc | 860.42 | K | Joback Method |

## Sources

**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=C36176315&Units=SI
**Crippen Method:** http://pubs.acs.org/doi/abs/10.1021/ci990307l
**Crippen Method:** https://www.chemeo.com/doc/models/crippen_log10ws

## 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 |