# 2-Biphenylisothiocyanate

**Inchi:** InChI=1S/C13H9NS/c15-10-14-13-9-5-4-8-12(13)11-6-2-1-3-7-11/h1-9H
**InchiKey:** OAYSYSIGKCDBKZ-UHFFFAOYSA-N
**Formula:** C13H9NS
**SMILES:** S=C=Nc1ccccc1-c1ccccc1
**Mol. weight [g/mol]:** 211.28
**CAS:** 19394-61-7

# Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| hf | 434.01 | kJ/mol | Joback Method |
| hvap | 60.19 | kJ/mol | Joback Method |
| log10ws | -4.99 | | Crippen Method |
| logp | 4.088 | | Crippen Method |
| mcvol | 164.240 | ml/mol | McGowan Method |
| pc | 3096.73 | kPa | Joback Method |
| tb | 701.13 | K | Joback Method |
| tc | 986.59 | 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=C19394617&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 |