# 2,4-Dimethylphenylisothiocyanate

**Inchi:** InChI=1S/C9H9NS/c1-7-3-4-9(10-6-11)8(2)5-7/h3-5H,1-2H3
**InchiKey:** HOHSBFCSOARUBF-UHFFFAOYSA-N
**Formula:** C9H9NS
**SMILES:** Cc1ccc(N=C=S)c(C)c1
**Mol. weight [g/mol]:** 163.25

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| af | 0.4134 | | Cheméo Relay (1.0) |
| gf | 252.06 | kJ/mol | Cheméo Relay (1.0, beta) |
| hf | 210.42 | kJ/mol | Cheméo Relay (1.0) |
| hvap | 60.13 | kJ/mol | Cheméo Relay (1.0) |
| ie | 8.11 | eV | Cheméo Relay (1.0) |
| log10ws | -3.90 | | Cheméo Relay (1.0) |
| logp | 3.038 | | Crippen Method |
| mcvol | 131.640 | ml/mol | McGowan Method |
| pc | 3231.98 | kPa | Joback Method |
| tb | 478.11 | K | Cheméo Relay (1.0) |
| tc | 757.81 | K | Cheméo Relay (1.0) |
| tf | 285.67 | K | Cheméo Relay (1.0) |
| vc | 0.456 | m3/kmol | Cheméo Relay (1.0) |

## Sources

**Crippen Method:** http://pubs.acs.org/doi/abs/10.1021/ci990307l
**Crippen Method:** https://www.chemeo.com/doc/models/crippen_log10ws
**Cheméo Relay (1.0):**
**Cheméo Relay (1.0, beta):**
**NIST Webbook:** http://webbook.nist.gov/cgi/cbook.cgi?ID=C39842018&Units=SI
**Joback Method:** https://en.wikipedia.org/wiki/Joback_method
**McGowan Method:** http://link.springer.com/article/10.1007/BF02311772

# Legend

| | |
|---|---|
| **af:** | Acentric Factor |
| **gf:** | Standard Gibbs free energy of formation |
| **hf:** | Enthalpy of formation at standard conditions |
| **hvap:** | Enthalpy of vaporization at standard conditions |
| **ie:** | Ionization energy |
| **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 |
| **tf:** | Normal melting (fusion) point |
| **vc:** | Critical Volume |