# o-tolylthiourea

**Inchi:** InChI=1S/C8H10N2S/c1-6-4-2-3-5-7(6)10-8(9)11/h2-5H,1H3,(H3,9,10,11)
**InchiKey:** ACLZYRNSDLQOIA-UHFFFAOYSA-N
**Formula:** C8H10N2S
**SMILES:** Cc1ccccc1NC(N)=S
**Mol. weight [g/mol]:** 166.24
**CAS:** 614-78-8

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | 392.16 | kJ/mol | Joback Method |
| hf | 250.37 | kJ/mol | Joback Method |
| hfus | 25.03 | kJ/mol | Joback Method |
| hvap | 60.15 | kJ/mol | Joback Method |
| ie | 8.20 | eV | NIST Webbook |
| log10ws | -2.74 | | Crippen Method |
| logp | 1.651 | | Crippen Method |
| mcvol | 131.830 | ml/mol | McGowan Method |
| pc | 4397.41 | kPa | Joback Method |
| tb | 606.84 | K | Joback Method |
| tc | 856.91 | K | Joback Method |
| tf | 389.05 | K | Joback Method |
| vc | 0.475 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 299.68 | J/mol×K | 606.84 | Joback Method |
| cpg | 310.93 | J/mol×K | 648.52 | Joback Method |
| cpg | 321.26 | J/mol×K | 690.20 | Joback Method |
| cpg | 330.76 | J/mol×K | 731.88 | Joback Method |
| cpg | 339.53 | J/mol×K | 773.56 | Joback Method |
| cpg | 347.64 | J/mol×K | 815.23 | Joback Method |
| cpg | 355.21 | J/mol×K | 856.91 | 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=C614788&Units=SI |
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |

# Legend

| | |
|---|---|
| **cpg:** | Ideal gas heat capacity |
| **gf:** | Standard Gibbs free energy of formation |
| **hf:** | Enthalpy of formation at standard conditions |
| **hfus:** | Enthalpy of fusion 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 |

Latest version available from:
https://www.chemeo.com/cid/110-030-5/o-tolylthiourea.pdf
Generated by Cheméo on 2024-11-06 04:12:58.277077217 +0000 UTC m=+5447240.914046465.
Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.