# Benzo[b]thiophene-2-carboxylic acid

**Other names:** benzothiophene-2-carboxylic acid
**Inchi:** InChI=1S/C9H6O2S/c10-9(11)8-5-6-3-1-2-4-7(6)12-8/h1-5H,(H,10,11)
**InchiKey:** DYSJMQABFPKAQM-UHFFFAOYSA-N
**Formula:** C9H6O2S
**SMILES:** O=C(O)c1cc2ccccc2s1
**Mol. weight [g/mol]:** 178.21

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| hf | -207.99 | kJ/mol | Cheméo Relay (1.0) |
| ie | 8.36 | eV | Cheméo Relay (1.0) |
| logp | 2.599 | | Crippen Method |
| mcvol | 122.540 | ml/mol | McGowan Method |
| tf | 468.58 | K | Cheméo Relay (1.0) |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| rhos | 1490.00 | kg/m3 | 298.15 | Experimental and computational thermochemical study of benzofuran, benzothiophene and indole derivatives |

## Sources

**Experimental and computational thermochemical study of benzofuran, benzothiophene and indole derivatives:** https://www.doi.org/10.1016/j.jct.2016.02.008
**NIST Webbook:** http://webbook.nist.gov/cgi/cbook.cgi?ID=C6314289&Units=SI
**McGowan Method:** http://link.springer.com/article/10.1007/BF02311772
**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):**

# Legend

| | |
|---|---|
| **hf:** | Enthalpy of formation at standard conditions |
| **ie:** | Ionization energy |
| **logp:** | Octanol/Water partition coefficient |
| **mcvol:** | McGowan's characteristic volume |
| **rhos:** | Solid Density |
| **tf:** | Normal melting (fusion) point |