# BENZENECARBOTHIOIC ACID

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|---|---|
| **Other names:** | Benzoic acid, thio- |
| | Benzoyl thiol |
| | Monothiobenzoic acid |
| | Thiobenzoic acid |
| | Acido mercaptobenzoico |
| **Inchi:** | InChI=1S/C7H6OS/c8-7(9)6-4-2-1-3-5-6/h1-5H,(H,8,9) |
| **InchiKey:** | UIJGNTRUPZPVNG-UHFFFAOYSA-N |
| **Formula:** | C7H6OS |
| **SMILES:** | O=C(S)c1ccccc1 |
| **Mol. weight [g/mol]:** | 138.19 |

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| af | 0.4452 | | Cheméo Relay (1.0) |
| gf | 20.94 | kJ/mol | Joback Method |
| hf | -54.70 | kJ/mol | Cheméo Relay (1.0) |
| hfus | 13.57 | kJ/mol | Joback Method |
| hvap | 70.60 | kJ/mol | Cheméo Relay (1.0) |
| ie | 9.00 | eV | NIST Webbook |
| ie | 9.60 | eV | NIST Webbook |
| log10ws | -2.41 | | Cheméo Relay (1.0) |
| logp | 1.757 | | Crippen Method |
| mcvol | 103.650 | ml/mol | McGowan Method |
| pc | 4876.56 | kPa | Joback Method |
| tb | 490.47 | K | Cheméo Relay (1.0) |
| tc | 754.36 | K | Cheméo Relay (1.0) |
| tf | 372.90 | K | Cheméo Relay (1.0) |
| vc | 0.349 | m3/kmol | Cheméo Relay (1.0) |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 194.06 | J/mol×K | 502.97 | Joback Method |
| cpg | 204.74 | J/mol×K | 544.68 | Joback Method |

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|---|---|---|---|---|
| cpg | 214.60 | J/mol×K | 586.40 | Joback Method |
| cpg | 223.67 | J/mol×K | 628.11 | Joback Method |
| cpg | 232.00 | J/mol×K | 669.82 | Joback Method |
| cpg | 239.61 | J/mol×K | 711.54 | Joback Method |
| cpg | 246.57 | J/mol×K | 753.25 | Joback Method |

# Sources

**Cheméo Relay (1.0):**

**Cheméo Relay (1.0, beta):**

**NIST Webbook:** http://webbook.nist.gov/cgi/cbook.cgi?ID=C98919&Units=SI

**Joback Method:** https://en.wikipedia.org/wiki/Joback_method

**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

# Legend

**af:** Acentric Factor
**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