# 4-Methoxycarbonylphenyl isothiocyanate

**Inchi:** InChI=1S/C9H7NO2S/c1-12-9(11)7-2-4-8(5-3-7)10-6-13/h2-5H,1H3
**InchiKey:** WIZODHILGBTPPA-UHFFFAOYSA-N
**Formula:** C9H7NO2S
**SMILES:** COC(=O)c1ccc(N=C=S)cc1
**Mol. weight [g/mol]:** 193.22
**CAS:** 3662-78-0

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| hf | 35.24 | kJ/mol | Joback Method |
| hvap | 58.16 | kJ/mol | Joback Method |
| log10ws | -2.63 | | Crippen Method |
| logp | 2.208 | | Crippen Method |
| mcvol | 139.080 | ml/mol | McGowan Method |
| pc | 3468.36 | kPa | Joback Method |
| tb | 659.22 | K | Joback Method |
| tc | 916.43 | K | Joback Method |

## Sources

**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=C3662780&Units=SI
**Crippen Method:** http://pubs.acs.org/doi/abs/10.1021/ci990307l
**Crippen Method:** https://www.chemeo.com/doc/models/crippen_log10ws

## 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 |

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