# 4-CH3SO2-C6H4-COOCH3

**Inchi:** InChI=1S/C9H10O4S/c1-13-9(10)7-3-5-8(6-4-7)14(2,11)12/h3-6H,1-2H3
**InchiKey:** GUGXKWUWYBKREL-UHFFFAOYSA-N
**Formula:** C9H10O4S
**SMILES:** COC(=O)c1ccc(S(C)(=O)=O)cc1
**Mol. weight [g/mol]:** 214.24
**CAS:** 22821-70-1

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| affp | 827.70 | kJ/mol | NIST Webbook |
| basg | 796.70 | kJ/mol | NIST Webbook |
| gf | -574.78 | kJ/mol | Joback Method |
| hf | -702.18 | kJ/mol | Joback Method |
| hfus | 26.88 | kJ/mol | Joback Method |
| hvap | 66.36 | kJ/mol | Joback Method |
| log10ws | -1.41 | | Crippen Method |
| logp | 0.877 | | Crippen Method |
| mcvol | 149.440 | ml/mol | McGowan Method |
| pc | 4082.92 | kPa | Joback Method |
| tb | 561.05 | K | Joback Method |
| tc | 770.42 | K | Joback Method |
| tf | 340.85 | K | Joback Method |
| vc | 0.582 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 333.82 | J/mol×K | 561.05 | Joback Method |
| cpg | 346.41 | J/mol×K | 595.94 | Joback Method |
| cpg | 358.29 | J/mol×K | 630.84 | Joback Method |
| cpg | 369.46 | J/mol×K | 665.73 | Joback Method |
| cpg | 379.90 | J/mol×K | 700.63 | Joback Method |
| cpg | 389.62 | J/mol×K | 735.52 | Joback Method |
| cpg | 398.61 | J/mol×K | 770.42 | 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=C22821701&Units=SI |
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |
| **Crippen Method:** | https://www.chemeo.com/doc/models/crippen_log10ws |

# Legend

| | |
|---|---|
| **affp:** | Proton affinity |
| **basg:** | Gas basicity |
| **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 |
| **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 |