# 3-Methyl-4-aminobenzenesulfonamide

**Inchi:** InChI=1S/C7H10N2O2S/c1-5-4-6(12(9,10)11)2-3-7(5)8/h2-4H,8H2,1H3,(H2,9,10,11)
**InchiKey:** IGQGXIVCGKMRAM-UHFFFAOYSA-N
**Formula:** C7H10N2O2S
**SMILES:** Cc1cc(S(N)(=O)=O)ccc1N
**Mol. weight [g/mol]:** 186.23
**CAS:** 53297-70-4

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| chs | -4166.00 | kJ/mol | NIST Webbook |
| gf | -234.43 | kJ/mol | Joback Method |
| hf | -359.99 | kJ/mol | Joback Method |
| hfs | -620.10 | kJ/mol | NIST Webbook |
| hfus | 28.92 | kJ/mol | Joback Method |
| hvap | 74.69 | kJ/mol | Joback Method |
| log10ws | -1.28 | | Crippen Method |
| logp | 0.225 | | Crippen Method |
| mcvol | 133.780 | ml/mol | McGowan Method |
| pc | 5739.21 | kPa | Joback Method |
| tb | 589.04 | K | Joback Method |
| tc | 818.58 | K | Joback Method |
| tf | 425.19 | K | Joback Method |
| vc | 0.503 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 313.36 | J/mol×K | 589.04 | Joback Method |
| cpg | 324.87 | J/mol×K | 627.30 | Joback Method |
| cpg | 335.60 | J/mol×K | 665.55 | Joback Method |
| cpg | 345.57 | J/mol×K | 703.81 | Joback Method |
| cpg | 354.78 | J/mol×K | 742.07 | Joback Method |
| cpg | 363.22 | J/mol×K | 780.32 | Joback Method |
| cpg | 370.90 | J/mol×K | 818.58 | 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=C53297704&Units=SI |
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |

# Legend

| | |
|---|---|
| **chs:** | Standard solid enthalpy of combustion |
| **cpg:** | Ideal gas heat capacity |
| **gf:** | Standard Gibbs free energy of formation |
| **hf:** | Enthalpy of formation at standard conditions |
| **hfs:** | Solid phase 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 |