# 1-Methyl-4-(1-methyl-ethnenylsulphonyl)benzene

**Inchi:** InChI=1S/C10H12O2S/c1-8(2)13(11,12)10-6-4-9(3)5-7-10/h4-7H,1H2,2-3H3
**InchiKey:** FNWOMDYVPDCDJB-UHFFFAOYSA-N
**Formula:** C10H12O2S
**SMILES:** C=C(C)S(=O)(=O)c1ccc(C)cc1
**Mol. weight [g/mol]:** 196.27
**CAS:** 67605-02-1

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| chs | -5966.80 ± 1.90 | kJ/mol | NIST Webbook |
| gf | -253.15 | kJ/mol | Joback Method |
| hf | -197.00 ± 3.00 | kJ/mol | NIST Webbook |
| hfs | -285.20 ± 2.00 | kJ/mol | NIST Webbook |
| hfus | 24.10 | kJ/mol | Joback Method |
| hsub | 89.00 ± 2.00 | kJ/mol | NIST Webbook |
| hvap | 58.84 | kJ/mol | Joback Method |
| log10ws | -2.83 | | Crippen Method |
| logp | 2.302 | | Crippen Method |
| mcvol | 151.790 | ml/mol | McGowan Method |
| pc | 3628.97 | kPa | Joback Method |
| tb | 504.20 | K | Joback Method |
| tc | 711.84 | K | Joback Method |
| tf | 264.24 | K | Joback Method |
| vc | 0.596 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 318.09 | J/mol×K | 504.20 | Joback Method |
| cpg | 332.57 | J/mol×K | 538.81 | Joback Method |
| cpg | 346.24 | J/mol×K | 573.41 | Joback Method |
| cpg | 359.11 | J/mol×K | 608.02 | Joback Method |
| cpg | 371.19 | J/mol×K | 642.63 | Joback Method |
| cpg | 382.51 | J/mol×K | 677.24 | Joback Method |

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|---|---|---|---|---|
| cpg | 393.08 | J/mol×K | 711.84 | Joback Method |

# Sources

| | |
|---|---|
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=C67605021&Units=SI |
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |
| **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 |

# 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 |
| **hsub:** | Enthalpy of sublimation 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 |