# Benzene,[2-(methylthio)ethenyl]-(Z)-

**Inchi:** InChI=1S/C9H10S/c1-10-8-7-9-5-3-2-4-6-9/h2-8H,1H3/b8-7-
**InchiKey:** BWRWWBWZSDMTFX-FPLPWBNLSA-N
**Formula:** C9H10S
**SMILES:** CSC=Cc1ccccc1
**Mol. weight [g/mol]:** 150.24
**CAS:** 35822-50-5

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | 250.65 | kJ/mol | Joback Method |
| hf | 166.53 | kJ/mol | Joback Method |
| hfus | 17.44 | kJ/mol | Joback Method |
| hvap | 44.68 | kJ/mol | Joback Method |
| ie | 7.75 | eV | NIST Webbook |
| ie | 8.75 | eV | NIST Webbook |
| log10ws | -3.09 | | Crippen Method |
| logp | 3.020 | | Crippen Method |
| mcvol | 125.960 | ml/mol | McGowan Method |
| pc | 3534.66 | kPa | Joback Method |
| tb | 504.94 | K | Joback Method |
| tc | 747.08 | K | Joback Method |
| tf | 246.93 | K | Joback Method |
| vc | 0.466 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 247.64 | J/mol×K | 504.94 | Joback Method |
| cpg | 261.50 | J/mol×K | 545.30 | Joback Method |
| cpg | 274.35 | J/mol×K | 585.65 | Joback Method |
| cpg | 286.25 | J/mol×K | 626.01 | Joback Method |
| cpg | 297.25 | J/mol×K | 666.37 | Joback Method |
| cpg | 307.41 | J/mol×K | 706.73 | Joback Method |
| cpg | 316.79 | J/mol×K | 747.08 | Joback Method |

# Sources

| | |
|---|---|
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=C35822505&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

| | |
|---|---|
| **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 |

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