# 3-Cl-4-CH3S-C6H3-CCH

**Inchi:** InChI=1S/C9H7ClS/c1-3-7-4-5-9(11-2)8(10)6-7/h1,4-6H,2H3
**InchiKey:** YMRAHBGPMBCMLR-UHFFFAOYSA-N
**Formula:** C9H7ClS
**SMILES:** C#Cc1ccc(SC)c(Cl)c1
**Mol. weight [g/mol]:** 182.67
**CAS:** 120136-30-3

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| affp | 868.60 | kJ/mol | NIST Webbook |
| basg | 836.10 | kJ/mol | NIST Webbook |
| gf | 362.31 | kJ/mol | Joback Method |
| hf | 302.53 | kJ/mol | Joback Method |
| hfus | 23.63 | kJ/mol | Joback Method |
| hvap | 50.29 | kJ/mol | Joback Method |
| log10ws | -3.60 | | Crippen Method |
| logp | 3.043 | | Crippen Method |
| mcvol | 133.900 | ml/mol | McGowan Method |
| pc | 3659.77 | kPa | Joback Method |
| tb | 538.29 | K | Joback Method |
| tc | 795.02 | K | Joback Method |
| tf | 353.94 | K | Joback Method |
| vc | 0.496 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 254.42 | J/mol×K | 538.29 | Joback Method |
| cpg | 265.37 | J/mol×K | 581.08 | Joback Method |
| cpg | 275.53 | J/mol×K | 623.87 | Joback Method |
| cpg | 284.94 | J/mol×K | 666.65 | Joback Method |
| cpg | 293.63 | J/mol×K | 709.44 | Joback Method |
| cpg | 301.63 | J/mol×K | 752.23 | Joback Method |
| cpg | 308.98 | J/mol×K | 795.02 | 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=C120136303&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 |