

## 2-Butene, 1-[(1-methylethyl)thio]-, (Z)-

**InChI:** InChI=1S/C7H14S/c1-4-5-6-8-7(2)3/h4-5,7H,6H2,1-3H3/b5-4-

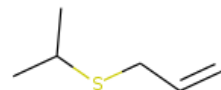
**InChI Key:** NBTBAEQTCSNSGX-PLNGDYQASA-N

**Formula:** C7H14S

**SMILES:** CC=CCSC(C)C

**Molecular Weight:** 130.25

**CAS:** 88915-94-0



### Physical Properties

| Property                        | Value   | Unit                   | Source         |
|---------------------------------|---------|------------------------|----------------|
| $\Delta_f G^\circ$              | 118.96  | kJ/mol                 | Joback Method  |
| $\Delta_f H^\circ_{\text{gas}}$ | -34.00  | kJ/mol                 | Joback Method  |
| $\Delta_{\text{fus}} H^\circ$   | 14.69   | kJ/mol                 | Joback Method  |
| $\Delta_{\text{vap}} H^\circ$   | 37.56   | kJ/mol                 | Joback Method  |
| $\log P_{\text{oct/wat}}$       | 2.70    |                        | Crippen Method |
| $P_c$                           | 3042.32 | kPa                    | Joback Method  |
| $T_{\text{boil}}$               | 432.06  | K                      | Joback Method  |
| $T_c$                           | 633.55  | K                      | Joback Method  |
| $T_{\text{fus}}$                | 182.97  | K                      | Joback Method  |
| $V_c$                           | 0.46    | m <sup>3</sup> /kg-mol | Joback Method  |

### Temperature Dependent Properties

| Property           | Value  | Unit    | Temperature (K) | Source        |
|--------------------|--------|---------|-----------------|---------------|
| $C_{p,\text{gas}}$ | 230.01 | J/mol×K | 432.06          | Joback Method |

### Sources

**Joback Method:** [https://en.wikipedia.org/wiki/Joback\\_method](https://en.wikipedia.org/wiki/Joback_method)

**NIST Webbook:**

[http://webbook.nist.gov/cgi/inchi/InChI=1S/C7H14S/c1-4-5-6-8-7\(2\)3/h4-5,7H,6H2,1-3H3/b5-4-](http://webbook.nist.gov/cgi/inchi/InChI=1S/C7H14S/c1-4-5-6-8-7(2)3/h4-5,7H,6H2,1-3H3/b5-4-)

**Crippen Method:** <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

## Legend

$C_{p, \text{gas}}$ : Ideal gas heat capacity (J/mol×K).

$\Delta_f G^\circ$ : Standard Gibbs free energy of formation (kJ/mol).

$\Delta_f H^\circ_{\text{gas}}$ : Enthalpy of formation at standard conditions (kJ/mol).

$\Delta_{\text{fus}} H^\circ$ : Enthalpy of fusion at standard conditions (kJ/mol).

$\Delta_{\text{vap}} H^\circ$ : Enthalpy of vaporization at standard conditions (kJ/mol).

$\log P_{\text{oct/wat}}$ : Octanol/Water partition coefficient .

$P_c$ : Critical Pressure (kPa).

$T_{\text{boil}}$ : Normal Boiling Point Temperature (K).

$T_c$ : Critical Temperature (K).

$T_{\text{fus}}$ : Normal melting (fusion) point (K).

$V_c$ : Critical Volume (m<sup>3</sup>/kg-mol).

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