

## 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-

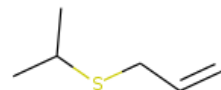
**InChI Key:** NBTBAEQTCSNSGX-PLNGDYQASA-N

**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

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

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

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

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

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

$logP_{oct/wat}$ : Octanol/Water partition coefficient .

$P_c$ : Critical Pressure (kPa).

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

$T_c$ : Critical Temperature (K).

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

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

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