

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-

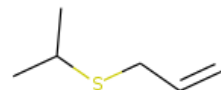
InChI Key: NBTBAEQTCSNSGX-PLNGDYQASA-N

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_{boil}	432.06	K	Joback Method
T_c	633.55	K	Joback Method
T_{fus}	182.97	K	Joback Method
V_c	0.46	m ³ /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

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

T_c : Critical Temperature (K).

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

V_c : Critical Volume (m³/kg-mol).

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