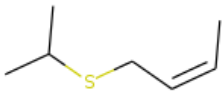
2-Butene, 1-[(1-methylethyl)thio]-, (Z)-

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
$\Delta_f G°$	118.96	kJ/mol	Joback Method
$\Delta_f H°_{gas}$	-34.00	kJ/mol	Joback Method
$\Delta_{fus} H°$	14.69	kJ/mol	Joback Method
$\Delta_{vap} H°$	37.56	kJ/mol	Joback Method
$log P_{oct/wat}$	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
$C_{p,gas}$	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-

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

$\mathbf{C_{p,gas}}$: Ideal gas heat capacity (J/mol×K).
$\mathbf{\Delta_f G°}$: Standard Gibbs free energy of formation (kJ/mol).
$\mathbf{\Delta_f H°_{gas}}$: Enthalpy of formation at standard conditions (kJ/mol).
$\mathbf{\Delta_{fus} H°}$: Enthalpy of fusion at standard conditions (kJ/mol).
$\mathbf{\Delta_{vap} H°}$: Enthalpy of vaporization at standard conditions (kJ/mol).
$\mathbf{\mathit{log}P_{oct/wat}}$: Octanol/Water partition coefficient .
$\mathbf{P_c}$: Critical Pressure (kPa).
$\mathbf{T_{boil}}$: Normal Boiling Point Temperature (K).
$\mathbf{T_c}$: Critical Temperature (K).
$\mathbf{T_{fus}}$: Normal melting (fusion) point (K).
$\mathbf{V_c}$: Critical Volume (m^3/kg-mol).