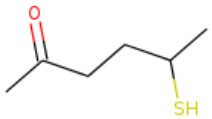
5-Mercaptohexan-2-one

InChI: InChI=1S/C6H12OS/c1-5(7)3-4-6(2)8/h6,8H,3-4H2,1-2H3
InChI Key: GFUOWPYWXSTOFZ-UHFFFAOYSA-N
Formula: C6H12OS
SMILES: CC(=O)CCC(C)S
Molecular Weight: 132.22



Physical Properties

Property	Value	Unit	Source
$\Delta_f G°$	-102.33	kJ/mol	Joback Method
$\Delta_f H°_{gas}$	-246.55	kJ/mol	Joback Method
$\Delta_{fus} H°$	13.41	kJ/mol	Joback Method
$\Delta_{vap} H°$	42.05	kJ/mol	Joback Method
$logP_{oct/wat}$	1.67		Crippen Method
P_c	3633.35	kPa	Joback Method
T_{boil}	452.97	K	Joback Method
T_c	658.46	K	Joback Method
T_{fus}	228.77	K	Joback Method
V_c	0.43	m^3/kg-mol	Joback Method

Temperature Dependent Properties

Property	Value	Unit	Temperature (K)	Source
$C_{p,gas}$	222.01	J/mol×K	452.97	Joback Method

Sources

Joback Method: https://en.wikipedia.org/wiki/Joback_method
NIST Webbook: http://webbook.nist.gov/cgi/inchi/InChI=1S/C6H12OS/c1-5(7)3-4-6(2)8/h6,8H,3-4H2,1-2H3
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

$\mathbf{C_{p,gas}}$: Ideal gas heat capacity (J/mol×K).
$\Delta_f\mathbf{G°}$: Standard Gibbs free energy of formation (kJ/mol).
$\Delta_f\mathbf{H°_{gas}}$: Enthalpy of formation at standard conditions (kJ/mol).
$\Delta_{fus}\mathbf{H°}$: Enthalpy of fusion at standard conditions (kJ/mol).
$\Delta_{vap}\mathbf{H°}$: Enthalpy of vaporization at standard conditions (kJ/mol).
$\boldsymbol{log}\mathbf{P_{oct/wat}}$: 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).