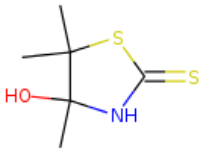
4-Hydroxy-4,5,5-trimethylthiazolidine-2-thione

InChI: InChI=1S/C6H11NOS2/c1-5(2)6(3,8)7-4(9)10-5/h8H,1-3H3,(H,7,9)
InChI Key: CFUUJNLSMDIFGY-UHFFFAOYSA-N
Formula: C6H11NOS2
SMILES: CC1(O)NC(=S)SC1(C)C
Molecular Weight: 177.29
CAS: 19975-64-5



Physical Properties

Property	Value	Unit	Source
$\Delta_f G°$	99.10	kJ/mol	Joback Method
$\Delta_f H°_{gas}$	-50.61	kJ/mol	Joback Method
$\Delta_{fus} H°$	17.08	kJ/mol	Joback Method
$\Delta_{vap} H°$	63.32	kJ/mol	Joback Method
$logP_{oct/wat}$	1.09		Crippen Method
P_c	5235.81	kPa	Joback Method
T_{boil}	608.97	K	Joback Method
T_c	849.84	K	Joback Method
T_{fus}	524.81	K	Joback Method
V_c	0.45	m^3/kg-mol	Joback Method

Temperature Dependent Properties

Property	Value	Unit	Temperature (K)	Source
$C_{p,gas}$	296.96	J/mol×K	608.97	Joback Method

Sources

Joback Method: https://en.wikipedia.org/wiki/Joback_method
NIST Webbook: http://webbook.nist.gov/cgi/inchi/InChI=1S/C6H11NOS2/c1-5(2)6(3,8)7-4(9)10-5/h8H,1-3H3,(H,7,9)
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).