trans-2,4-dimethyl-thiacyclopentane

InChI:
InChI=1S/C6H12S/c1-5-3-6(2)7-4-5/h5-6H,3-4H2,1-2H3/t5-,6-/m0/s1
InChI Key: YLAZTYUYPNOQJN-WDSKDSINSA-N
Formula: C6H12S
SMILES: CC1CSC(C)C1
Molecular Weight: 116.22

Physical Properties

Property	Value	Unit	Source
$\Delta_f G°$	68.34	kJ/mol	Joback Method
$\Delta_f H°_{gas}$	-81.77	kJ/mol	Joback Method
$\Delta_{fus} H°$	9.96	kJ/mol	Joback Method
$\Delta_{vap} H°$	34.71	kJ/mol	Joback Method
$logP_{oct/wat}$	2.15		Crippen Method
P_c	3659.77	kPa	Joback Method
T_{boil}	395.12	K	Joback Method
T_c	607.56	K	Joback Method
T_{fus}	247.49	K	Joback Method
V_c	0.36	m^3/kg-mol	Joback Method

Temperature Dependent Properties

Property	Value	Unit	Temperature (K)	Source
$C_{p,gas}$	182.26	J/mol×K	395.12	Joback Method

Sources

Joback Method: https://en.wikipedia.org/wiki/Joback_method
NIST Webbook: http://webbook.nist.gov/cgi/inchi/InChI=1S/C6H12S/c1-5-3-6(2)7-4-5/h5-6H,3-4H2,1-2H3/t5-,6-/m0/s1
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).