

trans-2,4-dimethyl-thiacyclopentane

InChI:

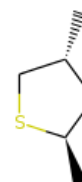
InChI=1S/C6H12S/c1-5-3-6(2)7-4-5/h5-6H,3-4H2,1-2H3/t5-,6-/m0/s1

InChI Key: YLAZTYUYPNQJN-WDSKDSINSA-N

Formula: C6H12S

SMILES: CC1CSC(C)C1

Molecular Weight: 116.22



Physical Properties

Property	Value	Unit	Source
$\Delta_f G^\circ$	68.34	kJ/mol	Joback Method
$\Delta_f H^\circ_{\text{gas}}$	-81.77	kJ/mol	Joback Method
$\Delta_{\text{fus}} H^\circ$	9.96	kJ/mol	Joback Method
$\Delta_{\text{vap}} H^\circ$	34.71	kJ/mol	Joback Method
$\log P_{\text{oct/wat}}$	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
$C_{p,\text{gas}}$	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](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/ci9903071>

Legend

$C_{p, gas}$: Ideal gas heat capacity (J/mol×K).

$\Delta_f G^\circ$: Standard Gibbs free energy of formation (kJ/mol).

$\Delta_f H^\circ_{gas}$: Enthalpy of formation at standard conditions (kJ/mol).

$\Delta_{fus} H^\circ$: Enthalpy of fusion at standard conditions (kJ/mol).

$\Delta_{vap} H^\circ$: Enthalpy of vaporization at standard conditions (kJ/mol).

$logP_{oct/wat}$: 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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