cis,trans-2,3,5-trimethyl-thiacyclopentane

Inchi: InChI=1S/C7H14S/c1-5-4-6(2)8-7(5)3/h5-7H,4H2,1-3H3/t5-,6-,7-/m0/s1
InchiKey: MLHOTFJTKPLNPX-ACZMJKKPSA-N
Formula: C7H14S
SMILES: CC1CC(C)C(C)S1
Mol. weight [g/mol]: 130.25

Physical Properties

Property code	Value	Unit	Source
gf	69.05	kJ/mol	Joback Method
hf	-122.75	kJ/mol	Joback Method
hfus	13.62	kJ/mol	Joback Method
hvap	36.63	kJ/mol	Joback Method
log10ws	-2.51		Crippen Method
logp	2.536		Crippen Method
mcvol	114.980	ml/mol	McGowan Method
pc	3149.09	kPa	Joback Method
rinpol	964.00		NIST Webbook
rinpol	964.00		NIST Webbook
rinpol	964.00		NIST Webbook
tb	413.33	K	Joback Method
tc	623.07	K	Joback Method
tf	254.52	K	Joback Method
vc	0.412	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	222.18	J/mol×K	413.33	Joback Method
cpg	238.25	J/mol×K	448.29	Joback Method
cpg	253.57	J/mol×K	483.24	Joback Method
cpg	268.15	J/mol×K	518.20	Joback Method
cpg	282.02	J/mol×K	553.16	Joback Method
cpg	295.20	J/mol×K	588.11	Joback Method
cpg	307.68	J/mol×K	623.07	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R208894&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume