2,2-dimethyl-thiacyclopentane

Inchi: InChI=1S/C6H12S/c1-6(2)4-3-5-7-6/h3-5H2,1-2H3
InchiKey: XUZUHHOTUSNHDJ-UHFFFAOYSA-N
Formula: C6H12S
SMILES: CC1(C)CCCS1
Mol. weight [g/mol]: 116.22

Physical Properties

Property code	Value	Unit	Source
gf	70.56	kJ/mol	Joback Method
hf	-46.19	kJ/mol	Joback Method
hfus	2.59	kJ/mol	Joback Method
hvap	33.87	kJ/mol	Joback Method
log10ws	-2.22		Crippen Method
logp	2.292		Crippen Method
mcvol	100.890	ml/mol	McGowan Method
pc	4031.24	kPa	Joback Method
rinpol	887.00		NIST Webbook
tb	400.03	K	Joback Method
tc	623.18	K	Joback Method
tf	275.63	K	Joback Method
vc	0.356	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	182.54	J/mol×K	400.03	Joback Method
cpg	197.57	J/mol×K	437.22	Joback Method
cpg	211.36	J/mol×K	474.41	Joback Method
cpg	224.04	J/mol×K	511.61	Joback Method
cpg	235.72	J/mol×K	548.80	Joback Method
cpg	246.55	J/mol×K	585.99	Joback Method
cpg	256.63	J/mol×K	623.18	Joback Method

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R208636&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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