2,2,5-trimethyl-thiacyclopentane

Inchi: InChI=1S/C7H14S/c1-6-4-5-7(2,3)8-6/h6H,4-5H2,1-3H3
InchiKey: DHIFJEDHXBEYEE-UHFFFAOYSA-N
Formula: C7H14S
SMILES: CC1CCC(C)(C)S1
Mol. weight [g/mol]: 130.25

Physical Properties

Property code	Value	Unit	Source
gf	71.27	kJ/mol	Joback Method
hf	-87.17	kJ/mol	Joback Method
hfus	6.25	kJ/mol	Joback Method
hvap	35.78	kJ/mol	Joback Method
log10ws	-2.75		Crippen Method
logp	2.680		Crippen Method
mcvol	114.980	ml/mol	McGowan Method
pc	3443.98	kPa	Joback Method
rinpol	905.00		NIST Webbook
tb	418.24	K	Joback Method
tc	638.26	K	Joback Method
tf	282.66	K	Joback Method
vc	0.411	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	222.73	J/mol×K	418.24	Joback Method
cpg	239.15	J/mol×K	454.91	Joback Method
cpg	254.36	J/mol×K	491.58	Joback Method
cpg	268.48	J/mol×K	528.25	Joback Method
cpg	281.63	J/mol×K	564.92	Joback Method
cpg	293.92	J/mol×K	601.59	Joback Method
cpg	305.47	J/mol×K	638.26	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=R208616&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