3,3-dimethyl-thiacyclohexane

Inchi: InChI=1S/C7H14S/c1-7(2)4-3-5-8-6-7/h3-6H2,1-2H3
InchiKey: VTTAITZGCXLKBP-UHFFFAOYSA-N
Formula: C7H14S
SMILES: CC1(C)CCCSC1
Mol. weight [g/mol]: 130.25

Physical Properties

Property code	Value	Unit	Source
gf	66.88	kJ/mol	Joback Method
hf	-72.99	kJ/mol	Joback Method
hfus	3.08	kJ/mol	Joback Method
hvap	36.27	kJ/mol	Joback Method
log10ws	-2.29		Crippen Method
logp	2.540		Crippen Method
mcvol	114.980	ml/mol	McGowan Method
pc	3690.97	kPa	Joback Method
rinpol	989.00		NIST Webbook
rinpol	989.00		NIST Webbook
tb	427.18	K	Joback Method
tc	657.02	K	Joback Method
tf	283.38	K	Joback Method
vc	0.405	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	221.23	J/mol×K	427.18	Joback Method
cpg	238.33	J/mol×K	465.49	Joback Method
cpg	254.12	J/mol×K	503.79	Joback Method
cpg	268.73	J/mol×K	542.10	Joback Method
cpg	282.29	J/mol×K	580.41	Joback Method
cpg	294.94	J/mol×K	618.71	Joback Method
cpg	306.79	J/mol×K	657.02	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R208696&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