2-ethyl-2-methyl-thiacyclopentane

Inchi: InChI=1S/C7H14S/c1-3-7(2)5-4-6-8-7/h3-6H2,1-2H3
InchiKey: HIYCBGXWUDZAKB-UHFFFAOYSA-N
Formula: C7H14S
SMILES: CCC1(C)CCCS1
Mol. weight [g/mol]: 130.25

Physical Properties

Property code	Value	Unit	Source
gf	78.98	kJ/mol	Joback Method
hf	-66.83	kJ/mol	Joback Method
hfus	5.18	kJ/mol	Joback Method
hvap	36.09	kJ/mol	Joback Method
log10ws	-2.64		Crippen Method
logp	2.682		Crippen Method
mcvol	114.980	ml/mol	McGowan Method
pc	3581.35	kPa	Joback Method
rinpol	994.00		NIST Webbook
rinpol	994.00		NIST Webbook
tb	422.91	K	Joback Method
tc	643.34	K	Joback Method
tf	286.90	K	Joback Method
vc	0.412	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	222.38	J/mol×K	422.91	Joback Method
cpg	238.45	J/mol×K	459.65	Joback Method
cpg	253.27	J/mol×K	496.39	Joback Method
cpg	266.99	J/mol×K	533.13	Joback Method
cpg	279.72	J/mol×K	569.86	Joback Method
cpg	291.58	J/mol×K	606.60	Joback Method
cpg	302.70	J/mol×K	643.34	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R208641&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

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