4,5-dehydro-2-methylthiacyclopentane

Inchi: InChI=1S/C5H8S/c1-5-3-2-4-6-5/h2,4-5H,3H2,1H3
InchiKey: MFAXBTKOLOJEHX-UHFFFAOYSA-N
Formula: C5H8S
SMILES: CC1CC=CS1
Mol. weight [g/mol]: 100.18

Physical Properties

Property code	Value	Unit	Source
gf	97.59	kJ/mol	Joback Method
hf	16.99	kJ/mol	Joback Method
hfus	7.52	kJ/mol	Joback Method
hvap	33.09	kJ/mol	Joback Method
log10ws	-2.15		Crippen Method
logp	2.026		Crippen Method
mcvol	82.500	ml/mol	McGowan Method
pc	4516.42	kPa	Joback Method
ripol	1108.00		NIST Webbook
ripol	1108.00		NIST Webbook
tb	376.07	K	Joback Method
tc	593.44	K	Joback Method
tf	241.22	K	Joback Method
vc	0.288	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	132.81	J/mol×K	376.07	Joback Method
cpg	144.23	J/mol×K	412.30	Joback Method
cpg	154.97	J/mol×K	448.53	Joback Method
cpg	165.07	J/mol×K	484.76	Joback Method
cpg	174.55	J/mol×K	520.99	Joback Method
cpg	183.44	J/mol×K	557.21	Joback Method
cpg	191.77	J/mol×K	593.44	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R298961&Units=SI

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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume