Hexathiepane

Other names: 1,2,3,4,5,6-Hexathiepane
Inchi: InChI=1S/CH2S6/c1-2-4-6-7-5-3-1/h1H2
InchiKey: JMYWPEQXUQGQNF-UHFFFAOYSA-N
Formula: CH2S6
SMILES: C1SSSSSS1
Mol. weight [g/mol]: 206.42
CAS: 17233-71-5

Physical Properties

Property code	Value	Unit	Source
gf	216.76	kJ/mol	Joback Method
hf	276.09	kJ/mol	Joback Method
hfus	8.95	kJ/mol	Joback Method
hvap	53.60	kJ/mol	Joback Method
log10ws	-4.88		Crippen Method
logp	3.932		Crippen Method
mcvol	112.190	ml/mol	McGowan Method
pc	8463.32	kPa	Joback Method
rinpol	1697.00		NIST Webbook
rinpol	1697.00		NIST Webbook
tb	537.75	K	Joback Method
tc	890.03	K	Joback Method
tf	609.83	K	Joback Method
vc	0.293	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	172.84	J/mol×K	537.75	Joback Method
cpg	179.86	J/mol×K	596.46	Joback Method
cpg	186.02	J/mol×K	655.18	Joback Method
cpg	191.42	J/mol×K	713.89	Joback Method
cpg	196.12	J/mol×K	772.60	Joback Method
cpg	200.19	J/mol×K	831.32	Joback Method

cpg	203.72	J/mol×K	890.03	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=C17233715&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume