Hexathiane

Other names:	Cyclohexasulfide
	Sulfur
	Cyclic hexaatomic sulfur
	Sulfur, S6
	Sulfur hexamer
	Cyclohexasulfur
Inchi:	InChI=1S/S6/c1-2-4-6-5-3-1
InchiKey:	FEXCMMPRRBSCRG-UHFFFAOYSA-N
Formula:	S6
SMILES:	S1SSSSS1
Mol. weight [g/mol]:	192.39
CAS:	13798-23-7

Physical Properties

Property code	Value	Unit	Source
ea	3.21 ± 0.07	eV	NIST Webbook
gf	220.44	kJ/mol	Joback Method
hf	302.89	kJ/mol	Joback Method
hfus	8.46	kJ/mol	Joback Method
hvap	51.20	kJ/mol	Joback Method
ie	8.50 ± 0.30	eV	NIST Webbook
ie	9.20 ± 0.20	eV	NIST Webbook
ie	9.70 ± 0.30	eV	NIST Webbook
ie	9.00 ± 0.03	eV	NIST Webbook
log10ws	-4.96		Crippen Method
logp	3.889		Crippen Method
mcvol	98.100	ml/mol	McGowan Method
pc	9687.52	kPa	Joback Method
rinpol	1499.20		NIST Webbook
tb	510.60	K	Joback Method
tc	858.34	K	Joback Method
tf	602.08	K	Joback Method
vc	0.245	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	136.19	J/mol×K	510.60	Joback Method
cpg	140.00	J/mol×K	568.56	Joback Method
cpg	143.21	J/mol×K	626.51	Joback Method
cpg	145.91	J/mol×K	684.47	Joback Method
cpg	148.19	J/mol×K	742.42	Joback Method
cpg	150.15	J/mol×K	800.38	Joback Method
cpg	151.88	J/mol×K	858.34	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=C13798237&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
ea:	Electron affinity
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
ie:	Ionization energy
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