1,2,3,4,6,7-Hexathiocane

Inchi: InChI=1S/C2H4S6/c1-3-4-2-6-8-7-5-1/h1-2H2
InchiKey: YGKDVYXUYSWNGO-UHFFFAOYSA-N
Formula: C2H4S6
SMILES: C1SSCSSSS1
Mol. weight [g/mol]: 220.44

Physical Properties

Property code	Value	Unit	Source
gf	213.08	kJ/mol	Joback Method
hf	249.29	kJ/mol	Joback Method
hfus	9.44	kJ/mol	Joback Method
hvap	56.00	kJ/mol	Joback Method
log10ws	-4.81		Crippen Method
logp	3.974		Crippen Method
mcvol	126.280	ml/mol	McGowan Method
pc	7457.32	kPa	Joback Method
rinpol	1864.00		NIST Webbook
tb	564.90	K	Joback Method
tc	921.06	K	Joback Method
tf	617.58	K	Joback Method
vc	0.342	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	212.61	J/mol×K	564.90	Joback Method
cpg	222.66	J/mol×K	624.26	Joback Method
cpg	231.59	J/mol×K	683.62	Joback Method
cpg	239.45	J/mol×K	742.98	Joback Method
cpg	246.30	J/mol×K	802.34	Joback Method
cpg	252.18	J/mol×K	861.70	Joback Method
cpg	257.16	J/mol×K	921.06	Joback Method

Sources

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=R587152&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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