1,2,3,4,5-Pentathiane

Inchi: InChI=1S/CH2S5/c1-2-4-6-5-3-1/h1H2
InchiKey: CLYCCGMFKNZNJJ-UHFFFAOYSA-N
Formula: CH2S5
SMILES: C1SSSSS1
Mol. weight [g/mol]: 174.35

Physical Properties

Property code	Value	Unit	Source
gf	189.00	kJ/mol	Joback Method
hf	236.99	kJ/mol	Joback Method
hfus	7.40	kJ/mol	Joback Method
hvap	47.62	kJ/mol	Joback Method
log10ws	-4.01		Crippen Method
logp	3.284		Crippen Method
mcvol	95.840	ml/mol	McGowan Method
pc	8175.04	kPa	Joback Method
rinpol	1418.00		NIST Webbook
tb	485.65	K	Joback Method
tc	806.14	K	Joback Method
tf	529.90	K	Joback Method
vc	0.256	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	142.69	J/mol×K	485.65	Joback Method
cpg	148.97	J/mol×K	539.07	Joback Method
cpg	154.52	J/mol×K	592.48	Joback Method
cpg	159.43	J/mol×K	645.90	Joback Method
cpg	163.76	J/mol×K	699.31	Joback Method
cpg	167.59	J/mol×K	752.73	Joback Method
cpg	170.99	J/mol×K	806.14	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=R587147&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