1,2,3,4,6-Pentathiepane

Inchi: InChI=1S/C2H4S5/c1-3-2-5-7-6-4-1/h1-2H2
InchiKey: VUWWZQBBXCOVBJ-UHFFFAOYSA-N
Formula: C2H4S5
SMILES: C1SCSSSS1
Mol. weight [g/mol]: 188.38

Physical Properties

Property code	Value	Unit	Source
gf	185.32	kJ/mol	Joback Method
hf	210.19	kJ/mol	Joback Method
hfus	7.89	kJ/mol	Joback Method
hvap	50.02	kJ/mol	Joback Method
log10ws	-3.93		Crippen Method
logp	3.326		Crippen Method
mcvol	109.930	ml/mol	McGowan Method
pc	7218.50	kPa	Joback Method
rinpol	1572.00		NIST Webbook
rinpol	1572.00		NIST Webbook
tb	512.80	K	Joback Method
tc	838.46	K	Joback Method
tf	537.65	K	Joback Method
vc	0.303	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	179.21	J/mol×K	512.80	Joback Method
cpg	188.51	J/mol×K	567.08	Joback Method
cpg	196.88	J/mol×K	621.35	Joback Method
cpg	204.37	J/mol×K	675.63	Joback Method
cpg	211.05	J/mol×K	729.91	Joback Method
cpg	216.98	J/mol×K	784.18	Joback Method
cpg	222.22	J/mol×K	838.46	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=R587167&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