1,2,4,5,7-Pentathiocane

Other names: 1,2,4,5,7-Pentathiaoctane
Inchi: InChI=1S/C3H6S5/c1-4-2-6-8-3-7-5-1/h1-3H2
InchiKey: QFHGOPGLIADNQA-UHFFFAOYSA-N
Formula: C3H6S5
SMILES: C1SCSSCSS1
Mol. weight [g/mol]: 202.41
CAS: 81531-39-7

Physical Properties

Property code	Value	Unit	Source
gf	181.64	kJ/mol	Joback Method
hf	183.39	kJ/mol	Joback Method
hfus	8.38	kJ/mol	Joback Method
hvap	52.41	kJ/mol	Joback Method
log10ws	-3.86		Crippen Method
logp	3.369		Crippen Method
mcvol	124.020	ml/mol	McGowan Method
pc	6420.53	kPa	Joback Method
rinpol	1749.00		NIST Webbook
tb	539.95	K	Joback Method
tc	870.11	K	Joback Method
tf	545.40	K	Joback Method
vc	0.351	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	218.90	J/mol×K	539.95	Joback Method
cpg	231.08	J/mol×K	594.98	Joback Method
cpg	242.09	J/mol×K	650.00	Joback Method
cpg	251.98	J/mol×K	705.03	Joback Method
cpg	260.78	J/mol×K	760.05	Joback Method
cpg	268.56	J/mol×K	815.08	Joback Method
cpg	275.35	J/mol×K	870.11	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=C81531397&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
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