1,3,5,7-Tetrathiocane

Other names: 1,3,5,7-Tetrathiacyclooctane
1,3,5,7-Tetrathiocyclooctane
Inchi: InChI=1S/C4H8S4/c1-5-2-7-4-8-3-6-1/h1-4H2
InchiKey: QRGGVNODEBZTBI-UHFFFAOYSA-N
Formula: C4H8S4
SMILES: C1SCSCSCS1
Mol. weight [g/mol]: 184.37
CAS: 2373-00-4

Physical Properties

Property code	Value	Unit	Source
gf	150.20	kJ/mol	Joback Method
hf	117.49	kJ/mol	Joback Method
hfus	7.31	kJ/mol	Joback Method
hvap	48.83	kJ/mol	Joback Method
ie	7.80	eV	NIST Webbook
ie	8.37	eV	NIST Webbook
log10ws	-2.91		Crippen Method
logp	2.763		Crippen Method
mcvol	121.760	ml/mol	McGowan Method
pc	5585.83	kPa	Joback Method
rinpol	1518.00		NIST Webbook
rinpol	1518.00		NIST Webbook
tb	515.00	K	Joback Method
tc	820.50	K	Joback Method
tf	473.22	K	Joback Method
vc	0.361	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	222.70	J/mol×K	515.00	Joback Method
cpg	236.80	J/mol×K	565.92	Joback Method
cpg	249.72	J/mol×K	616.83	Joback Method

cpg	261.49	J/mol×K	667.75	Joback Method
cpg	272.16	J/mol×K	718.66	Joback Method
cpg	281.76	J/mol×K	769.58	Joback Method
cpg	290.34	J/mol×K	820.50	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=C2373004&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
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