trithiocarbonic acid

Inchi: InChI=1S/CH2S3/c2-1(3)4/h(H2,2,3,4)
InchiKey: HIZCIEIDIFGZSS-UHFFFAOYSA-N
Formula: CH2S3
SMILES: S=C(S)S
Mol. weight [g/mol]: 110.22
CAS: 594-08-1

Physical Properties

Property code	Value	Unit	Source
gf	133.38	kJ/mol	Joback Method
hf	159.49	kJ/mol	Joback Method
hfl	24.00 ± 1.50	kJ/mol	NIST Webbook
hfus	11.03	kJ/mol	Joback Method
hvap	38.02	kJ/mol	Joback Method
log10ws	-1.73		Crippen Method
logp	1.131		Crippen Method
mcvol	69.700	ml/mol	McGowan Method
pc	8355.36	kPa	Joback Method
sl	218.00	J/mol×K	NIST Webbook
tb	418.04	K	Joback Method
tc	683.22	K	Joback Method
tf	246.30 ± 0.50	K	NIST Webbook
vc	0.235	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	102.74	J/mol×K	594.83	Joback Method
cpg	104.60	J/mol×K	639.02	Joback Method
cpg	91.72	J/mol×K	418.04	Joback Method
cpg	95.13	J/mol×K	462.24	Joback Method
cpg	98.06	J/mol×K	506.43	Joback Method
cpg	100.58	J/mol×K	550.63	Joback Method
cpg	106.23	J/mol×K	683.22	Joback Method

cpl	146.50	J/mol×K	273.00	NIST Webbook
hfust	8.41	kJ/mol	246.30	NIST Webbook
sfust	34.10	J/mol×K	246.30	NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C594081&Units=SI
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

Legend

cpg:	Ideal gas heat capacity
cpl:	Liquid phase heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfl:	Liquid phase enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hfust:	Enthalpy of fusion at a given temperature
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
sfust:	Entropy of fusion at a given temperature
sl:	Liquid phase molar entropy at standard conditions
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume