1,3,5-Trithiane

Other names:	s-Trithiane
	Formaldehyde, thio-, trimer
	Trimethylene trisulfide
	Trithioformaldehyde
	1,3,5-Trithiacyclohexane
	sym-Trithiane
	sym-Trithian
	Thioform
	Trimethylentrisulfid
	NSC 1937
Inchi:	InChI=1S/C3H6S3/c1-4-2-6-3-5-1/h1-3H2
InchiKey:	LORRLQMLLQLPSJ-UHFFFAOYSA-N
Formula:	C3H6S3
SMILES:	C1SCSCS1
Mol. weight [g/mol]:	138.28
CAS:	291-21-4

Physical Properties

Property code	Value	Unit	Source
gf	126.12	kJ/mol	Joback Method
hf	105.19	kJ/mol	Joback Method
hfus	5.26	kJ/mol	Joback Method
hsub	93.20 ± 0.20	kJ/mol	NIST Webbook
hsub	93.90	kJ/mol	NIST Webbook
hvap	40.45	kJ/mol	Joback Method
ie	7.70	eV	NIST Webbook
ie	8.76	eV	NIST Webbook
ie	8.83 ± 0.05	eV	NIST Webbook
ie	8.58	eV	NIST Webbook
log10ws	-2.11		Crippen Method
logp	2.072		Crippen Method
mcvol	91.320	ml/mol	McGowan Method
pc	6046.69	kPa	Joback Method
rinpol	1271.00		NIST Webbook
rinpol	1259.00		NIST Webbook
rinpol	1271.00		NIST Webbook
rinpol	1271.00		NIST Webbook

tb	435.75	K	Joback Method
tc	706.04	K	Joback Method
tf	385.54	K	Joback Method
vc	0.276	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	147.83	J/mol×K	435.75	Joback Method
cpg	158.30	J/mol×K	480.80	Joback Method
cpg	167.94	J/mol×K	525.85	Joback Method
cpg	176.80	J/mol×K	570.89	Joback Method
cpg	184.93	J/mol×K	615.94	Joback Method
cpg	192.38	J/mol×K	660.99	Joback Method
cpg	199.19	J/mol×K	706.04	Joback Method
hfust	32.20	kJ/mol	488.40	NIST Webbook
hsubt	91.50	kJ/mol	329.50	NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C291214&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
gf: Standard Gibbs free energy of formation
hf: Enthalpy of formation at standard conditions
hfus: Enthalpy of fusion at standard conditions
hfust: Enthalpy of fusion at a given temperature
hsub: Enthalpy of sublimation at standard conditions
hsubt: Enthalpy of sublimation at a given temperature

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