1,3-Dithiane-2-thione

Other names:	1,3-Dithian-2-thione
	m-Dithiane-2-thione
	Carbonic acid, trithio-, cyclic trimethylene ester
	Trimethylene trithiocarbonate
	1,3-Dithiacyclohexane-2-thione
	1,3-Propanedithiol, cyclic carbonotrithioate
	1,3-Propanedithiol, cyclic trithioacrbonate
Inchi:	InChI=1S/C4H6S3/c5-4-6-2-1-3-7-4/h1-3H2
InchiKey:	BVNLWJVULAZODX-UHFFFAOYSA-N
Formula:	C4H6S3
SMILES:	S=C1SCCCS1
Mol. weight [g/mol]:	150.28
CAS:	1748-15-8

Physical Properties

Property code	Value	Unit	Source
chg	-4224.60 ± 0.40	kJ/mol	NIST Webbook
gf	185.53	kJ/mol	Joback Method
hf	77.50 ± 2.70	kJ/mol	NIST Webbook
hfus	10.23	kJ/mol	Joback Method
hsub	91.40 ± 2.50	kJ/mol	NIST Webbook
hvap	91.00 ± 3.00	kJ/mol	NIST Webbook
ie	8.20	eV	NIST Webbook
ie	8.40	eV	NIST Webbook
log10ws	-2.51		Crippen Method
logp	2.141		Crippen Method
mcvol	101.110	ml/mol	McGowan Method
pc	5809.41	kPa	Joback Method
tb	483.44	K	Joback Method
tc	757.39	K	Joback Method
tf	377.03	K	Joback Method
vc	0.324	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	173.99	J/mol×K	483.44	Joback Method
cpg	184.01	J/mol×K	529.10	Joback Method
cpg	193.10	J/mol×K	574.76	Joback Method
cpg	201.34	J/mol×K	620.41	Joback Method
cpg	208.82	J/mol×K	666.07	Joback Method
cpg	215.63	J/mol×K	711.73	Joback Method
cpg	221.85	J/mol×K	757.39	Joback Method
hsubt	88.60	kJ/mol	334.50	NIST Webbook

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=C1748158&Units=SI

Legend

chg: Standard gas enthalpy of combustion
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
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
tb: Normal Boiling Point Temperature

tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume