Tetrathiafulvalene

Other names:	1,3-Dithiole, 2-(1,3-dithiol-2-ylidene)-
	1,4,5,8-Tetrathiafulvalene
	«DELTA»2,2'-Bi-1,3-dithiole
	«delta»-2:2'-bis(1,3-dithiazole)
	Â«DELTAÂ»2,2'-Bi-1,3-dithiole
	Â«deltaÂ»-2:2'-bis(1,3-dithiazole)
Inchi:	InChI=1S/C6H4S4/c1-2-8-5(7-1)6-9-3-4-10-6/h1-4H
InchiKey:	FHCPAXDKURNIOZ-UHFFFAOYSA-N
Formula:	C6H4S4
SMILES:	C1=CSC(=C2SC=CS2)S1
Mol. weight [g/mol]:	204.36
CAS:	31366-25-3

Physical Properties

Property code	Value	Unit	Source
chs	-5619.50 ± 1.70	kJ/mol	NIST Webbook
gf	318.22	kJ/mol	Joback Method
hf	325.91	kJ/mol	Joback Method
hfs	290.80 ± 1.70	kJ/mol	NIST Webbook
hfus	14.54	kJ/mol	Joback Method
hvap	55.53	kJ/mol	Joback Method
ie	6.83	eV	NIST Webbook
ie	6.83	eV	NIST Webbook
ie	7.00	eV	NIST Webbook
ie	6.72	eV	NIST Webbook
ie	6.92 ± 0.03	eV	NIST Webbook
ie	6.30	eV	NIST Webbook
log10ws	-5.18		Crippen Method
logp	4.015		Crippen Method
mcvol	126.180	ml/mol	McGowan Method
pc	5791.74	kPa	Joback Method
tb	575.34	K	Joback Method
tc	890.86	K	Joback Method
tf	548.78	K	Joback Method
vc	0.398	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	270.74	J/mol×K	838.27	Joback Method
cpg	231.96	J/mol×K	575.34	Joback Method
cpg	241.66	J/mol×K	627.93	Joback Method
cpg	250.21	J/mol×K	680.51	Joback Method
cpg	257.80	J/mol×K	733.10	Joback Method
cpg	264.59	J/mol×K	785.69	Joback Method
cpg	276.43	J/mol×K	890.86	Joback Method
hsubt	95.00 ± 1.00	kJ/mol	345.00	NIST Webbook
hsubt	92.00 ± 6.30	kJ/mol	351.00	NIST Webbook
hvapt	95.30	kJ/mol	343.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	2.10780e+01
Coeff. B	-9.44085e+03
Coeff. C	-2.45000e+00
Temperature range (K), min.	456.55
Temperature range (K), max.	601.24

Sources

The Yaws Handbook of Vapor Pressure: https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

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=C31366253&Units=SI

Legend

chs:	Standard solid enthalpy of combustion
cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfs:	Solid phase enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hsubt:	Enthalpy of sublimation at a given temperature
hvap:	Enthalpy of vaporization at standard conditions
hvapt:	Enthalpy of vaporization at a given temperature
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
pvap:	Vapor pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume