Thiirane

Other names:	2,3-Dihydrothiirene ETHYLENE EPISULFIDE ETHYLENE SULFIDE Ethylene episulphide Ethylene sulphide NSC 89690 THIIRENE Thiacyclopropane Thiirene, 2,3-dihydro- epithioethane
Inchi:	InChI=1S/C2H4S/c1-2-3-1/h1-2H2
InchiKey:	VOVUARRWDCVURC-UHFFFAOYSA-N
Formula:	C2H4S
SMILES:	C1CS1
Mol. weight [g/mol]:	60.12
CAS:	420-12-2

Physical Properties

Property code	Value	Unit	Source
af	0.1540		KDB
affp	807.40	kJ/mol	NIST Webbook
basg	777.60	kJ/mol	NIST Webbook
chl	-2012.60	kJ/mol	NIST Webbook
gf	74.28	kJ/mol	Joback Method
hf	82.30 ± 1.00	kJ/mol	NIST Webbook
hfl	52.00 ± 1.00	kJ/mol	NIST Webbook
hfus	1.66	kJ/mol	Joback Method
hvap	30.30 ± 0.20	kJ/mol	NIST Webbook
hvap	30.30	kJ/mol	NIST Webbook
ie	9.05	eV	NIST Webbook
ie	8.87 ± 0.15	eV	NIST Webbook
ie	9.05 ± 0.01	eV	NIST Webbook
ie	9.00	eV	NIST Webbook
ie	9.00	eV	NIST Webbook
ie	9.05	eV	NIST Webbook
ie	9.04 ± 0.01	eV	NIST Webbook
ie	8.90 ± 0.10	eV	NIST Webbook

ie	8.90	eV	NIST Webbook
log10ws	-0.44		Crippen Method
logp	0.733		Crippen Method
mcvol	44.530	ml/mol	McGowan Method
pc	7380.00	kPa	KDB
rinpol	589.00		NIST Webbook
rinpol	588.00		NIST Webbook
rinpol	606.00		NIST Webbook
rinpol	588.00		NIST Webbook
rinpol	606.00		NIST Webbook
ripol	899.00		NIST Webbook
tb	329.00 ± 3.00	K	NIST Webbook
tb	328.70	K	NIST Webbook
tb	328.10	K	KDB
tb	328.90 ± 0.50	K	NIST Webbook
tc	555.00	K	KDB
tf	165.00	K	KDB
vc	0.151	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	53.14	J/mol×K	304.40	Joback Method
cpg	59.39	J/mol×K	337.57	Joback Method
cpg	65.13	J/mol×K	370.74	Joback Method
cpg	70.39	J/mol×K	403.91	Joback Method
cpg	75.23	J/mol×K	437.09	Joback Method
cpg	79.65	J/mol×K	470.26	Joback Method
cpg	83.71	J/mol×K	503.43	Joback Method
hvapt	29.20	kJ/mol	328.10	KDB
hvapt	30.50	kJ/mol	326.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.43596e+01

Coeff. B	-2.85218e+03
Coeff. C	-3.59060e+01
Temperature range (K), min.	238.59
Temperature range (K), max.	351.13

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	6.49904e+01
Coeff. B	-5.61461e+03
Coeff. C	-7.58624e+00
Coeff. D	6.41076e-06
Temperature range (K), min.	238.15
Temperature range (K), max.	555.00

Sources

Joback Method: https://en.wikipedia.org/wiki/Joback_method

KDB: https://www.cheric.org/files/research/kdb/mol/mol1858.mol

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C420122&Units=SI

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

KDB Vapor Pressure Data: https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1858

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

af: Acentric Factor

affp: Proton affinity

basg: Gas basicity

chl: Standard liquid enthalpy of combustion

cpg: Ideal gas 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

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
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume