3-Ethylthio-1-propene

Other names:	4-Thia-1-hexene
	Allyl ethyl sulfide
	Allyl ethyl sulphide
	CH2=CHCH2SC2H5
Inchi:	InChI=1S/C5H10S/c1-3-5-6-4-2/h3H,1,4-5H2,2H3
InchiKey:	NOJXPGXFDASWEI-UHFFFAOYSA-N
Formula:	C5H10S
SMILES:	C=CCSCC
Mol. weight [g/mol]:	102.20
CAS:	5296-62-8

Physical Properties

Property code	Value	Unit	Source
chl	-3977.40 ± 1.90	kJ/mol	NIST Webbook
gf	112.18	kJ/mol	Joback Method
hf	18.00 ± 3.00	kJ/mol	NIST Webbook
hfl	-21.00 ± 3.00	kJ/mol	NIST Webbook
hfus	11.56	kJ/mol	Joback Method
hvap	39.00 ± 1.00	kJ/mol	NIST Webbook
hvap	39.00	kJ/mol	NIST Webbook
hvap	39.30	kJ/mol	NIST Webbook
ie	8.51 ± 0.01	eV	NIST Webbook
log10ws	-1.65		Crippen Method
logp	1.925		Crippen Method
mcvol	93.360	ml/mol	McGowan Method
pc	3722.56	kPa	Joback Method
rinpol	777.00		NIST Webbook
rinpol	777.00		NIST Webbook
tb	379.26	K	Joback Method
tc	573.61	K	Joback Method
tf	178.75	K	Joback Method
vc	0.350	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	155.70	J/mol×K	379.26	Joback Method
cpg	165.05	J/mol×K	411.65	Joback Method
cpg	174.01	J/mol×K	444.04	Joback Method
cpg	182.59	J/mol×K	476.44	Joback Method
cpg	190.80	J/mol×K	508.83	Joback Method
cpg	198.64	J/mol×K	541.22	Joback Method
cpg	206.14	J/mol×K	573.61	Joback Method
hvapt	38.90	kJ/mol	313.50	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	7.01322e+00
Coeff. B	-5.54504e+02
Coeff. C	-2.05297e+02
Temperature range (K), min.	287.74
Temperature range (K), max.	531.14

Sources

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C5296628&Units=SI

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

Legend

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