Sulfide, ethyl propyl

Other names:	1-(ETHYLTHIO)PROPANE
	3-THIAHEXANE
	ETHYL PROPYL THIO ETHER
	Ethyl n-propyl sulfide
	Ethyl propyl sulfide
	Ethyl propyl sulphide
	Ethyl propyl thioether
	Propane, 1-(ethylthio)-
	Propyl ethyl sulfide
	n-C3H7SC2H5
Inchi:	InChI=1S/C5H12S/c1-3-5-6-4-2/h3-5H2,1-2H3
InchiKey:	ZDDDFDQTSXYYSE-UHFFFAOYSA-N
Formula:	C5H12S
SMILES:	CCCSCC
Mol. weight [g/mol]:	104.21
CAS:	4110-50-3

Physical Properties

Property code	Value	Unit	Source
chl	-4139.90 ± 0.59	kJ/mol	NIST Webbook
chl	-4139.50 ± 0.59	kJ/mol	NIST Webbook
gf	24.34	kJ/mol	Joback Method
hf	-104.50	kJ/mol	NIST Webbook
hf	-104.70 ± 0.79	kJ/mol	NIST Webbook
hfl	-144.60 ± 0.75	kJ/mol	NIST Webbook
hfl	-144.80 ± 0.79	kJ/mol	NIST Webbook
hfus	12.84	kJ/mol	Joback Method
hvap	40.10 ± 0.04	kJ/mol	NIST Webbook
hvap	39.50	kJ/mol	NIST Webbook
hvap	40.10	kJ/mol	NIST Webbook
hvap	40.01	kJ/mol	NIST Webbook
hvap	40.08	kJ/mol	NIST Webbook
hvap	40.00	kJ/mol	NIST Webbook
ie	8.50 ± 0.05	eV	NIST Webbook
ie	8.37	eV	NIST Webbook
log10ws	-1.80		Crippen Method
logp	2.150		Crippen Method

mcvol	97.660	ml/mol	McGowan Method
pc	3538.87	kPa	Joback Method
rinpol	782.00		NIST Webbook
rinpol	785.00		NIST Webbook
rinpol	801.00		NIST Webbook
rinpol	783.00		NIST Webbook
rinpol	785.00		NIST Webbook
rinpol	794.00		NIST Webbook
rinpol	794.00		NIST Webbook
rinpol	794.00		NIST Webbook
rinpol	785.00		NIST Webbook
ripol	1017.00		NIST Webbook
ripol	1017.00		NIST Webbook
sl	309.53	J/mol×K	NIST Webbook
tb	391.70 ± 0.30	K	NIST Webbook
tb	391.70	K	NIST Webbook
tb	391.70	K	NIST Webbook
tb	389.00 ± 3.00	K	NIST Webbook
tc	572.69	K	Joback Method
tf	156.11 ± 0.10	K	NIST Webbook
tt	156.10 ± 0.04	K	NIST Webbook
tt	156.10 ± 0.03	K	NIST Webbook
vc	0.369	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	169.71	J/mol×K	382.58	Joback Method
cpg	224.63	J/mol×K	572.69	Joback Method
cpg	216.36	J/mol×K	541.00	Joback Method
cpg	207.75	J/mol×K	509.32	Joback Method
cpg	198.78	J/mol×K	477.63	Joback Method
cpg	189.45	J/mol×K	445.95	Joback Method
cpg	179.76	J/mol×K	414.26	Joback Method
cpl	198.41	J/mol×K	298.15	NIST Webbook
hfust	10.58	kJ/mol	156.10	NIST Webbook
hfust	10.58	kJ/mol	156.10	NIST Webbook
hfust	10.58	kJ/mol	156.10	NIST Webbook
hvapt	34.24	kJ/mol	391.70	NIST Webbook
hvapt	37.80	kJ/mol	364.50	NIST Webbook
hvapt	39.80	kJ/mol	355.50	NIST Webbook

sfust	67.78	J/mol×K	156.10	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.42227e+01
Coeff. B	-3.21450e+03
Coeff. C	-5.70070e+01
Temperature range (K), min.	287.68
Temperature range (K), max.	417.73

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	9.12345e+01
Coeff. B	-7.82974e+03
Coeff. C	-1.13601e+01
Coeff. D	7.81191e-06
Temperature range (K), min.	287.15
Temperature range (K), max.	584.00

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

KDB: https://www.cheric.org/files/research/kdb/mol/mol1832.mol

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C4110503&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=1832

Legend

chl:	Standard liquid enthalpy of combustion
cpg:	Ideal gas heat capacity
cpl:	Liquid phase 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
hfust:	Enthalpy of fusion 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
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
sfust:	Entropy of fusion at a given temperature
sl:	Liquid phase molar entropy at standard conditions
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
tt:	Triple Point Temperature
vc:	Critical Volume