Propane, 2-(ethylthio)-

Other names:	2-(Ethylthio)propane
	2-Methyl-3-thiapentane
	C2H5S(iso-C3H7)
	Ethyl isopropyl sulfide
	Ethyl isopropyl sulphide
	Isopropyl ethyl sulfide
	Isopropyl ethyl sulphide
	Sulfide, ethyl isopropyl
Inchi:	InChI=1S/C5H12S/c1-4-6-5(2)3/h5H,4H2,1-3H3
InchiKey:	NZUQQADVSXWVNW-UHFFFAOYSA-N
Formula:	C5H12S
SMILES:	CCSC(C)C
Mol. weight [g/mol]:	104.21
CAS:	5145-99-3

Physical Properties

Property code	Value	Unit	Source
chl	-4128.30 ± 2.00	kJ/mol	NIST Webbook
gf	21.90	kJ/mol	Joback Method
hf	-117.00 ± 3.00	kJ/mol	NIST Webbook
hfl	-156.00 ± 2.00	kJ/mol	NIST Webbook
hfus	9.31	kJ/mol	Joback Method
hvap	37.90 ± 0.80	kJ/mol	NIST Webbook
hvap	38.50	kJ/mol	NIST Webbook
hvap	37.80	kJ/mol	NIST Webbook
hvap	39.00 ± 1.00	kJ/mol	NIST Webbook
hvap	39.00	kJ/mol	NIST Webbook
ie	8.35 ± 0.01	eV	NIST Webbook
log10ws	-1.91		Crippen Method
logp	2.148		Crippen Method
mcvol	97.660	ml/mol	McGowan Method
pc	3572.80	kPa	Joback Method
rinpol	746.00		NIST Webbook
rinpol	739.00		NIST Webbook
rinpol	754.00		NIST Webbook
rinpol	746.00		NIST Webbook
rinpol	746.00		NIST Webbook

rinpol	746.00		NIST Webbook
tb	380.50 ± 0.30	K	NIST Webbook
tb	376.00 ± 3.00	K	NIST Webbook
tc	576.94	K	Joback Method
tf	150.96 ± 0.10	K	NIST Webbook
vc	0.363	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	199.69	J/mol×K	479.54	Joback Method
cpg	208.93	J/mol×K	512.01	Joback Method
cpg	217.80	J/mol×K	544.47	Joback Method
cpg	169.65	J/mol×K	382.14	Joback Method
cpg	180.05	J/mol×K	414.61	Joback Method
cpg	190.07	J/mol×K	447.07	Joback Method
cpg	226.28	J/mol×K	576.94	Joback Method
hvapt	38.10	kJ/mol	345.00	NIST Webbook
hvapt	36.30	kJ/mol	355.00	NIST Webbook
hvapt	38.10	kJ/mol	310.50	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.36233e+01
Coeff. B	-2.87663e+03
Coeff. C	-6.10480e+01
Temperature range (K), min.	276.76
Temperature range (K), max.	407.14

Sources

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=C5145993&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

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