Propane, 1-(methylthio)-

Other names:	1-(Methylthio)propane
	2-Thiapentane
	METHYL N-PROPYL SULFIDE
	Methyl propyl sulfide
	Methyl propyl sulphide
	Sulfide, methyl propyl
	n-C3H7SCH3
Inchi:	InChI=1S/C4H10S/c1-3-4-5-2/h3-4H2,1-2H3
InchiKey:	ZOASGOXWEHUTKZ-UHFFFAOYSA-N
Formula:	C4H10S
SMILES:	CCCSC
Mol. weight [g/mol]:	90.19
CAS:	3877-15-4

Physical Properties

Property code	Value	Unit	Source
gf	15.92	kJ/mol	Joback Method
hf	-84.02	kJ/mol	Joback Method
hfus	10.25	kJ/mol	Joback Method
hvap	36.31	kJ/mol	NIST Webbook
hvap	36.30 ± 0.40	kJ/mol	NIST Webbook
hvap	36.20	kJ/mol	NIST Webbook
ie	8.80 ± 0.15	eV	NIST Webbook
log10ws	-1.38		Crippen Method
logp	1.759		Crippen Method
mcvol	83.570	ml/mol	McGowan Method
pc	3980.54	kPa	Joback Method
rinpol	752.00		NIST Webbook
rinpol	714.00		NIST Webbook
rinpol	705.00		NIST Webbook
rinpol	701.00		NIST Webbook
rinpol	702.00		NIST Webbook
rinpol	717.00		NIST Webbook
rinpol	715.00		NIST Webbook
rinpol	712.00		NIST Webbook
rinpol	715.00		NIST Webbook
rinpol	715.00		NIST Webbook

rinpol	718.00		NIST Webbook
rinpol	715.00		NIST Webbook
rinpol	723.00		NIST Webbook
rinpol	727.00		NIST Webbook
rinpol	707.00		NIST Webbook
rinpol	706.00		NIST Webbook
ripol	951.00		NIST Webbook
sl	272.55	J/mol×K	NIST Webbook
tb	368.80 ± 0.30	K	NIST Webbook
tb	368.80 ± 0.30	K	NIST Webbook
tb	368.70	K	NIST Webbook
tb	368.70	K	NIST Webbook
tb	367.00 ± 3.00	K	NIST Webbook
tc	574.10	K	NIST Webbook
tf	160.17 ± 0.10	K	NIST Webbook
tf	160.18 ± 0.06	K	NIST Webbook
tt	160.17 ± 0.05	K	NIST Webbook
vc	0.314	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	182.04	J/mol×K	550.75	Joback Method
cpg	143.93	J/mol×K	391.54	Joback Method
cpg	152.12	J/mol×K	423.38	Joback Method
cpg	160.03	J/mol×K	455.23	Joback Method
cpg	167.65	J/mol×K	487.07	Joback Method
cpg	174.99	J/mol×K	518.91	Joback Method
cpg	135.44	J/mol×K	359.70	Joback Method
cpl	171.63	J/mol×K	298.15	NIST Webbook
hfust	9.91	kJ/mol	160.20	NIST Webbook
hfust	9.91	kJ/mol	160.20	NIST Webbook
hfust	9.91	kJ/mol	160.17	NIST Webbook
hvapt	32.08	kJ/mol	368.70	NIST Webbook
hvapt	35.30	kJ/mol	341.00	NIST Webbook
hvapt	34.50 ± 0.10	kJ/mol	328.00	NIST Webbook
hvapt	33.40 ± 0.10	kJ/mol	347.00	NIST Webbook
hvapt	32.10 ± 0.10	kJ/mol	369.00	NIST Webbook
sfust	61.88	J/mol×K	160.17	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.42307e+01
Coeff. B	-3.05990e+03
Coeff. C	-5.03700e+01
Temperature range (K), min.	269.83
Temperature range (K), max.	393.44

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	8.08044e+01
Coeff. B	-6.94795e+03
Coeff. C	-9.86974e+00
Coeff. D	7.27846e-06
Temperature range (K), min.	269.15
Temperature range (K), max.	563.00

Sources

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C3877154&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=1823

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/mol1823.mol

Legend

cpg: Ideal gas heat capacity

cpl:	Liquid phase heat capacity
gf:	Standard Gibbs free energy of formation
hf:	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