Propyl mercaptan

Other names:	1-Mercaptopropane
	1-PROPANETHIOL
	1-Propyl mercaptan
	1-Propylthiol
	3-MERCAPTOPROPANOL
	N-PROPYL MERCAPTAN
	PROPANETHIOL
	Propane-1-thiol
	Propylthiol
	n-C3H7SH
	n-Propylthiol
Inchi:	InChI=1S/C3H8S/c1-2-3-4/h4H,2-3H2,1H3
InchiKey:	SUVIGLJNEAMWEG-UHFFFAOYSA-N
Formula:	C3H8S
SMILES:	CCCS
Mol. weight [g/mol]:	76.16
CAS:	107-03-9

Physical Properties

Property code	Value	Unit	Source
affp	794.90	kJ/mol	NIST Webbook
basg	763.60	kJ/mol	NIST Webbook
chl	-2825.30 ± 0.49	kJ/mol	NIST Webbook
gf	3.77	kJ/mol	Joback Method
hf	-68.58 ± 0.63	kJ/mol	NIST Webbook
hfl	-100.60 ± 0.63	kJ/mol	NIST Webbook
hfus	7.57	kJ/mol	Joback Method
hvap	32.00	kJ/mol	NIST Webbook
hvap	31.99	kJ/mol	NIST Webbook
hvap	32.05	kJ/mol	NIST Webbook
hvap	31.90	kJ/mol	NIST Webbook
ie	9.20 ± 0.01	eV	NIST Webbook
ie	9.21	eV	NIST Webbook
ie	9.20 ± 0.01	eV	NIST Webbook
ie	9.19	eV	NIST Webbook
log10ws	-1.15		Crippen Method
logp	1.326		Crippen Method

mcvol	69.480	ml/mol	McGowan Method
pc	4809.16	kPa	Joback Method
rhoc	265.80 ± 7.62	kg/m3	NIST Webbook
rinpol	594.00		NIST Webbook
rinpol	586.00		NIST Webbook
rinpol	617.00		NIST Webbook
rinpol	614.00		NIST Webbook
rinpol	596.00		NIST Webbook
rinpol	579.00		NIST Webbook
rinpol	600.00		NIST Webbook
rinpol	617.00		NIST Webbook
rinpol	630.00		NIST Webbook
rinpol	615.40		NIST Webbook
rinpol	615.70		NIST Webbook
rinpol	623.00		NIST Webbook
rinpol	586.00		NIST Webbook
rinpol	590.00		NIST Webbook
rinpol	619.00		NIST Webbook
rinpol	603.00		NIST Webbook
rinpol	600.00		NIST Webbook
rinpol	615.00		NIST Webbook
rinpol	614.00		NIST Webbook
rinpol	600.00		NIST Webbook
rinpol	587.00		NIST Webbook
rinpol	624.00		NIST Webbook
rinpol	617.00		NIST Webbook
rinpol	609.00		NIST Webbook
rinpol	616.00		NIST Webbook
rinpol	594.00		NIST Webbook
rinpol	601.00		NIST Webbook
rinpol	600.00		NIST Webbook
rinpol	614.00		NIST Webbook
rinpol	605.00		NIST Webbook
rinpol	623.00		NIST Webbook
ripol	817.00		NIST Webbook
ripol	840.00		NIST Webbook
ripol	830.00		NIST Webbook
ripol	857.00		NIST Webbook
ripol	857.00		NIST Webbook
ripol	840.00		NIST Webbook
ripol	843.00		NIST Webbook
ripol	845.00		NIST Webbook
ripol	833.00		NIST Webbook
ripol	855.00		NIST Webbook

sl	242.50	J/mol×K	NIST Webbook
tb	341.00 ± 1.38	K	NIST Webbook
tb	341.00 ± 3.00	K	NIST Webbook
tb	341.00 ± 3.00	K	NIST Webbook
tb	340.00 ± 2.00	K	NIST Webbook
tb	341.40 ± 1.00	K	NIST Webbook
tb	389.00 ± 3.00	K	NIST Webbook
tb	340.90	K	KDB
tb	340.70	K	NIST Webbook
tb	340.90	K	NIST Webbook
tb	338.00 ± 2.00	K	NIST Webbook
tb	340.95 ± 0.20	K	NIST Webbook
tb	340.70 ± 1.00	K	NIST Webbook
tb	341.00 ± 5.00	K	NIST Webbook
tb	341.00 ± 0.20	K	NIST Webbook
tb	340.97 ± 0.30	K	NIST Webbook
tb	342.00 ± 3.00	K	NIST Webbook
tb	340.97 ± 0.20	K	NIST Webbook
tb	340.50 ± 0.50	K	NIST Webbook
tb	340.90 ± 0.70	K	NIST Webbook
tb	340.70 ± 3.00	K	NIST Webbook
tb	341.00 ± 3.00	K	NIST Webbook
tb	335.00 ± 3.00	K	NIST Webbook
tc	536.60 ± 0.40	K	NIST Webbook
tc	536.60	K	KDB
tc	535.60	K	NIST Webbook
tf	159.80	K	KDB
tf	159.90 ± 0.30	K	NIST Webbook
tf	160.09 ± 0.10	K	NIST Webbook
tf	161.65 ± 0.50	K	NIST Webbook
tf	160.02 ± 0.02	K	NIST Webbook
tf	160.02 ± 0.10	K	NIST Webbook
tf	160.02 ± 0.10	K	NIST Webbook
tt	159.98 ± 0.05	K	NIST Webbook
tt	159.99 ± 0.03	K	NIST Webbook
tt	160.00 ± 0.07	K	NIST Webbook
vc	0.286	m3/kmol	KDB

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source

cpg	103.03	J/mol×K	330.90	Joback Method
cpg	122.76	J/mol×K	426.39	Joback Method
cpg	116.44	J/mol×K	394.56	Joback Method
cpg	109.87	J/mol×K	362.73	Joback Method
cpg	140.24	J/mol×K	521.88	Joback Method
cpg	134.65	J/mol×K	490.05	Joback Method
cpg	128.83	J/mol×K	458.22	Joback Method
cpl	144.56	J/mol×K	298.15	NIST Webbook
hfust	3.97	kJ/mol	142.10	NIST Webbook
hfust	5.48	kJ/mol	160.00	NIST Webbook
hfust	5.48	kJ/mol	160.00	NIST Webbook
hvapt	30.70 ± 0.10	kJ/mol	320.00	NIST Webbook
hvapt	31.60 ± 0.10	kJ/mol	303.00	NIST Webbook
hvapt	31.80	kJ/mol	336.00	NIST Webbook
hvapt	33.70	kJ/mol	309.00	NIST Webbook
hvapt	31.50	kJ/mol	312.00	NIST Webbook
hvapt	29.50 ± 0.10	kJ/mol	341.00	NIST Webbook
hvapt	29.54	kJ/mol	340.90	NIST Webbook
rfi	1.43530		298.15	Vapor Liquid Equilibrium for Methoxymethane + Thiophene, + Diethylsulfide, + 2-Methyl-2-propanethiol and 1-Hexene, + 1-Propanethiol
rfi	1.43530		298.15	Vapor-Liquid Equilibrium for Binary System of 1-Propanethiol, Thiophene, and Diethyl Sulfide with Toluene at 90.03 kPa
sfust	34.23	J/mol×K	160.00	NIST Webbook
sfust	27.95	J/mol×K	142.10	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.43731e+01
Coeff. B	-2.95656e+03
Coeff. C	-3.78120e+01
Temperature range (K), min.	247.71

Temperature range (K), max.	536.60

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	7.86939e+01
Coeff. B	-6.33433e+03
Coeff. C	-9.68363e+00
Coeff. D	8.41181e-06
Temperature range (K), min.	159.95
Temperature range (K), max.	536.00

Sources

Measurement of Henry s Law Constants and Infinite Dilution Activity Coefficients of Propyl Mercaptan, Butyl Mercaptan, and Dimethyl Sulfide in Methyldiethanolamine (1) + Water (2) with w1) 0.50 Using a Gas Stripping Technique:	https://www.doi.org/10.1021/je050268b
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
Infinite dilution activity coefficient measurements by inert gas stripping method:	https://www.doi.org/10.1016/j.fluid.2006.02.022
KDB Vapor Pressure Data:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1816
KDB:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1816
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C107039&Units=SI
Vapor-Liquid Equilibrium for Binary System of 1-Propanethiol, Thiophene, and Diethyl Sulfide with Toluene at 90.00 kPa:	https://www.doi.org/10.1021/je060093l
Measurement through a Gas Stripping Technique of Henry's Law Constants and Infinite Dilution Activity Coefficients of Propyl Mercaptan, Butyl Mercaptan, and Dimethyl Sulfide in Methyldiethanolamine (1) + Water (2) with w1 = 0.25 and 0.35:	https://www.doi.org/10.1021/je800349p
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
Phase Equilibrium Measurements and Modeling of 1-Propanethiol + Butanethiol + n-Butane Ternary System at 303, 336, and 368 K and Pressure Up to 9 MPa:	https://www.doi.org/10.1021/acs.jced.5b00134
Wilhoit Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Vapor Liquid Equilibrium for Methoxymethane + Thiophene, + Dimethylsulfide, + 2-Methyl-2-propanethiol and 1-Hexene, + 1-Propanethiol:	https://www.doi.org/10.1021/je3013028
Vapor-Liquid Equilibrium Measurements and Modeling of the Propyl Mercaptan + Methane + Water System:	https://www.doi.org/10.1021/je900441f

Legend

affp:	Proton affinity
basg:	Gas basicity
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
rfi:	Refractive Index
rhoc:	Critical density
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