Methanethiol

Other names:	CH3SH
	MERCAPTOMETHANE
	METHYL MERCAPTAN
	METHYL THIOALCOHOL
	Mercaptan methylique
	Methaanthiol
	Methanethiole
	Methanthiol
	Methvtiolo
	Methyl sulfhydrate
	Methylmercaptaan
	Metilmercaptano
	Rcra waste number U153
	Thiomethanol
	UN 1064
Inchi:	InChI=1S/CH4S/c1-2/h2H,1H3
InchiKey:	LSDPWZHWYPCBBB-UHFFFAOYSA-N
Formula:	CH4S
SMILES:	CS
Mol. weight [g/mol]:	48.11
CAS:	74-93-1

Physical Properties

Property code	Value	Unit	Source
af	0.1530		KDB
affp	773.40	kJ/mol	NIST Webbook
basg	742.00	kJ/mol	NIST Webbook
chl	-1520.80 ± 0.50	kJ/mol	NIST Webbook
dm	1.30	debye	KDB
gf	-9.92	kJ/mol	KDB
hf	-22.80 ± 0.59	kJ/mol	NIST Webbook
hf	-22.99	kJ/mol	KDB
hfl	-46.65 ± 0.54	kJ/mol	NIST Webbook
hfpi	889.00 ± 8.00	kJ/mol	NIST Webbook
hfpiz	898.00 ± 8.00	kJ/mol	NIST Webbook
hfus	2.39	kJ/mol	Joback Method
hvap	23.90	kJ/mol	NIST Webbook

hvap	23.80 ± 0.08	kJ/mol	NIST Webbook
hvap	23.80	kJ/mol	NIST Webbook
ie	9.45 ± 0.01	eV	NIST Webbook
ie	9.44	eV	NIST Webbook
ie	9.44 ± 0.00	eV	NIST Webbook
ie	9.44 ± 0.01	eV	NIST Webbook
ie	9.44 ± 0.01	eV	NIST Webbook
ie	9.42	eV	NIST Webbook
ie	9.44	eV	NIST Webbook
ie	9.44	eV	NIST Webbook
ie	9.44	eV	NIST Webbook
ie	9.46	eV	NIST Webbook
ie	9.44	eV	NIST Webbook
ie	9.44 ± 0.01	eV	NIST Webbook
ie	9.41	eV	NIST Webbook
log10ws	-0.31		Crippen Method
logp	0.546		Crippen Method
mcvol	41.300	ml/mol	McGowan Method
pc	7230.00 ± 50.66	kPa	NIST Webbook
pc	7230.00	kPa	KDB
rhoc	331.51 ± 1.92	kg/m3	NIST Webbook
rinpol	398.00		NIST Webbook
rinpol	460.00		NIST Webbook
rinpol	414.00		NIST Webbook
rinpol	400.00		NIST Webbook
rinpol	414.00		NIST Webbook
rinpol	400.00		NIST Webbook
rinpol	401.00		NIST Webbook
rinpol	401.00		NIST Webbook
rinpol	393.00		NIST Webbook
rinpol	396.00		NIST Webbook
rinpol	398.00		NIST Webbook
rinpol	401.00		NIST Webbook
rinpol	464.00		NIST Webbook
rinpol	464.00		NIST Webbook
rinpol	473.00		NIST Webbook
rinpol	414.00		NIST Webbook
rinpol	414.00		NIST Webbook
rinpol	460.00		NIST Webbook
rinpol	430.00		NIST Webbook
rinpol	444.00		NIST Webbook
rinpol	461.00		NIST Webbook
rinpol	414.00		NIST Webbook
ripol	696.00		NIST Webbook

ripol	640.00		NIST Webbook
ripol	688.00		NIST Webbook
ripol	695.00		NIST Webbook
ripol	694.00		NIST Webbook
ripol	690.00		NIST Webbook
ripol	690.00		NIST Webbook
ripol	643.00		NIST Webbook
ripol	643.00		NIST Webbook
ripol	699.00		NIST Webbook
ripol	700.00		NIST Webbook
ripol	688.00		NIST Webbook
ripol	702.00		NIST Webbook
ripol	702.00		NIST Webbook
ripol	702.00		NIST Webbook
ripol	699.00		NIST Webbook
ripol	679.00		NIST Webbook
ripol	668.00		NIST Webbook
ripol	655.00		NIST Webbook
ripol	702.00		NIST Webbook
ripol	675.00		NIST Webbook
sl	163.22	J/mol×K	NIST Webbook
tb	279.00 ± 2.00	K	NIST Webbook
tb	279.00 ± 3.00	K	NIST Webbook
tb	279.05 ± 0.10	K	NIST Webbook
tb	279.00 ± 2.00	K	NIST Webbook
tb	279.70 ± 0.50	K	NIST Webbook
tb	279.11	K	KDB
tb	279.00 ± 2.00	K	NIST Webbook
tc	470.00	K	KDB
tc	469.90 ± 0.40	K	NIST Webbook
tc	469.90 ± 0.40	K	NIST Webbook
tf	150.10 ± 0.50	K	NIST Webbook
tf	150.18 ± 0.02	K	NIST Webbook
tf	152.15 ± 0.60	K	NIST Webbook
tf	150.00	K	KDB
tf	150.10 ± 0.40	K	NIST Webbook
tt	150.16 ± 0.03	K	NIST Webbook
tt	150.14 ± 0.05	K	NIST Webbook
vc	0.145	m3/kmol	KDB
zc	0.2682700		KDB
zra	0.28		KDB

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	57.49	J/mol×K	380.07	Joback Method
cpg	51.70	J/mol×K	316.78	Joback Method
cpg	54.65	J/mol×K	348.42	Joback Method
cpg	65.49	J/mol×K	474.99	Joback Method
cpg	62.92	J/mol×K	443.35	Joback Method
cpg	60.25	J/mol×K	411.71	Joback Method
cpg	48.67	J/mol×K	285.14	Joback Method
cpl	89.04	J/mol×K	280.00	NIST Webbook
hfust	5.90	kJ/mol	150.20	NIST Webbook
hfust	5.90	kJ/mol	150.20	NIST Webbook
hfust	2.20	kJ/mol	137.60	NIST Webbook
hvapt	25.20	kJ/mol	313.00	NIST Webbook
hvapt	24.20	kJ/mol	442.00	NIST Webbook
hvapt	23.70	kJ/mol	384.50	NIST Webbook
hvapt	25.70	kJ/mol	252.00	NIST Webbook
hvapt	24.56	kJ/mol	279.10	KDB
hvapt	24.57	kJ/mol	279.12	NIST Webbook
hvapt	25.80	kJ/mol	250.50	NIST Webbook
hvapt	27.20	kJ/mol	253.00	NIST Webbook
pvap	42.00	kPa	258.00	Measurement of VLE (TPx or TPxy data) for hydrogen sulfide + (dimethylsulfide or ethylmethylsulfide or carbon disulfide) and methane solubilities in (dimethylsulfide or ethylmethylsulfide or methylmercaptan or ethylmercaptan)

pvap	80.00	kPa	272.98	Measurement of VLE (TPx or TPxy data) for hydrogen sulfide + (dimethylsulfide or ethylmethylsulfide or carbon disulfide) and methane solubilities in (dimethylsulfide or ethylmethylsulfide or methylmercaptan or ethylmercaptan)
pvap	170.00	kPa	293.35	Measurement of VLE (TPx or TPxy data) for hydrogen sulfide + (dimethylsulfide or ethylmethylsulfide or carbon disulfide) and methane solubilities in (dimethylsulfide or ethylmethylsulfide or methylmercaptan or ethylmercaptan)
pvap	20.00	kPa	243.19	Measurement of VLE (TPx or TPxy data) for hydrogen sulfide + (dimethylsulfide or ethylmethylsulfide or carbon disulfide) and methane solubilities in (dimethylsulfide or ethylmethylsulfide or methylmercaptan or ethylmercaptan)

pvap	200.00	kPa	298.23	Measurement of VLE (TPx or TPxy data) for hydrogen sulfide + (dimethylsulfide or ethylmethylsulfide or carbon disulfide) and methane solubilities in (dimethylsulfide or ethylmethylsulfide or methylmercaptan or ethylmercaptan)
rhol	866.00	kg/m3	293.00	KDB
sfust	39.33	J/mol×K	150.20	NIST Webbook
sfust	1.59	J/mol×K	137.60	NIST Webbook
srf	0.02	N/m	293.20	KDB
svapt	88.02	J/mol×K	279.12	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.42712e+01
Coeff. B	-2.32325e+03
Coeff. C	-3.84210e+01
Temperature range (K), min.	204.56
Temperature range (K), max.	429.95

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	9.18684e+01
Coeff. B	-5.80626e+03
Coeff. C	-1.19968e+01
Coeff. D	1.44187e-05
Temperature range (K), min.	150.18
Temperature range (K), max.	470.00

Sources

KDB:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1811
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
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=1811
Phase Equilibria of Three Binary Mixtures: Methanethiol + Methane, Methanethiol + Nitrogen, and Methanethiol + Carbon Dioxide:	https://www.doi.org/10.1021/je2011049
Gas-liquid partition coefficients and Henry's law constants of methyl mercaptan in aqueous solutions of Fe(II) CDTA chelate complex:	https://www.doi.org/10.1016/j.fluid.2007.02.008
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Measurement of VLE (TPx or TPxy data) for hydrogen sulfide + (dimethylsulfide or ethylmethylsulfide or carbon disulfide) and methane solubilities in (dimethylsulfide or ethylmethylsulfide or methylmercaptan or ethylmercaptan):	https://www.doi.org/10.1016/j.fluid.2007.07.013
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C74931&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

af:	Acentric Factor
affp:	Proton affinity
basg:	Gas basicity
chl:	Standard liquid enthalpy of combustion
cpg:	Ideal gas heat capacity
cpl:	Liquid phase heat capacity
dm:	Dipole Moment
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfl:	Liquid phase enthalpy of formation at standard conditions
hfpi:	Enthalpy of formation of positive ion at standard conditions
hfpiz:	Enthalpy of formation of positive ion at 0K
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
rhoc:	Critical density

rhol:	Liquid 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
srf:	Surface Tension
svapt:	Entropy of vaporization at a given temperature
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
tt:	Triple Point Temperature
vc:	Critical Volume
zc:	Critical Compressibility
zra:	Rackett Parameter