Ethane, (methylthio)-

Other names:	(METHYLTHIO)ETHANE
	1-(Methylsulfanyl)ethane
	1-(methylthio)ethane
	2-THIABUTANE
	C2H5SCH3
	Ethyl methyl sulfide
	Ethyl methyl sulphide
	METHYL ETHYL SULFIDE
	Methyl ethyl sulphide
	Sulfide, ethyl methyl
Inchi:	InChI=1S/C3H8S/c1-3-4-2/h3H2,1-2H3
InchiKey:	WXEHBUMAEPOYKP-UHFFFAOYSA-N
Formula:	C3H8S
SMILES:	CCSC
Mol. weight [g/mol]:	76.16
CAS:	624-89-5

Physical Properties

Property code	Value	Unit	Source
af	0.2160		KDB
affp	846.50	kJ/mol	NIST Webbook
basg	815.30	kJ/mol	NIST Webbook
chl	-2833.60 ± 1.10	kJ/mol	NIST Webbook
gf	11.40	kJ/mol	KDB
hf	-60.30 ± 1.10	kJ/mol	NIST Webbook
hf	-59.66	kJ/mol	KDB
hfl	-92.30 ± 1.10	kJ/mol	NIST Webbook
hfus	7.66	kJ/mol	Joback Method
hvap	31.50	kJ/mol	NIST Webbook
hvap	31.80	kJ/mol	NIST Webbook
hvap	31.99	kJ/mol	NIST Webbook
hvap	32.00	kJ/mol	NIST Webbook
ie	8.54	eV	NIST Webbook
ie	8.46	eV	NIST Webbook
ie	10.96	eV	NIST Webbook
ie	8.50 ± 0.10	eV	NIST Webbook
ie	8.55 ± 0.01	eV	NIST Webbook

ie	8.55 ± 0.01	eV	NIST Webbook
log10ws	-0.96		Crippen Method
logp	1.369		Crippen Method
mcvol	69.480	ml/mol	McGowan Method
pc	4260.00	kPa	KDB
rinpol	638.20		NIST Webbook
rinpol	621.90		NIST Webbook
rinpol	616.00		NIST Webbook
rinpol	608.00		NIST Webbook
rinpol	616.00		NIST Webbook
rinpol	623.00		NIST Webbook
rinpol	609.00		NIST Webbook
rinpol	618.80		NIST Webbook
rinpol	625.00		NIST Webbook
rinpol	619.00		NIST Webbook
rinpol	622.00		NIST Webbook
rinpol	620.00		NIST Webbook
rinpol	610.00		NIST Webbook
rinpol	614.00		NIST Webbook
rinpol	622.00		NIST Webbook
rinpol	625.00		NIST Webbook
rinpol	605.00		NIST Webbook
rinpol	617.00		NIST Webbook
rinpol	625.00		NIST Webbook
rinpol	608.00		NIST Webbook
rinpol	611.00		NIST Webbook
rinpol	609.00		NIST Webbook
ripol	859.00		NIST Webbook
ripol	829.00		NIST Webbook
ripol	859.00		NIST Webbook
ripol	859.00		NIST Webbook
tb	339.80	K	KDB
tb	339.80	K	NIST Webbook
tb	339.80	K	NIST Webbook
tb	335.20 ± 1.50	K	NIST Webbook
tb	339.80 ± 0.30	K	NIST Webbook
tb	340.00 ± 5.00	K	NIST Webbook
tc	533.00	K	KDB
tc	553.00	K	NIST Webbook
tf	167.20	K	KDB
tf	167.24 ± 0.10	K	NIST Webbook
tt	167.23 ± 0.02	K	NIST Webbook
vc	0.258	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	103.79	J/mol×K	336.82	Joback Method
cpg	110.56	J/mol×K	368.75	Joback Method
cpg	117.12	J/mol×K	400.67	Joback Method
cpg	123.47	J/mol×K	432.60	Joback Method
cpg	129.61	J/mol×K	464.53	Joback Method
cpg	135.54	J/mol×K	496.46	Joback Method
cpg	141.26	J/mol×K	528.38	Joback Method
hfust	9.76	kJ/mol	167.20	NIST Webbook
hfust	9.76	kJ/mol	167.20	NIST Webbook
hvapt	30.30	kJ/mol	338.00	NIST Webbook
hvapt	29.53	kJ/mol	339.80	NIST Webbook
hvapt	33.70	kJ/mol	308.00	NIST Webbook
hvapt	29.50	kJ/mol	340.20	KDB
hvapt	32.30	kJ/mol	287.00	NIST Webbook
hvapt	32.00 ± 0.08	kJ/mol	301.00	NIST Webbook
hvapt	31.64	kJ/mol	301.66	NIST Webbook
hvapt	31.80	kJ/mol	334.50	NIST Webbook
pvap	1.00	kPa	247.76	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	6.00	kPa	272.96	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	17.00	kPa	293.23	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)	
pvap	17.00	kPa	293.41	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	40.00	kPa	313.33	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	40.00	kPa	313.35	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)
rhol	837.00	kg/m3	293.00	KDB
srf	0.03	N/m	293.20	KDB

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.39945e+01
Coeff. B	-2.73161e+03
Coeff. C	-4.84660e+01
Temperature range (K), min.	247.75
Temperature range (K), max.	533.00

Information	Value
Property code	pvap

Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	7.85436e+01
Coeff. B	-6.34327e+03
Coeff. C	-9.63519e+00
Coeff. D	7.77843e-06
Temperature range (K), min.	247.15
Temperature range (K), max.	532.80

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C624895&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
KDB:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1818
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
KDB Vapor Pressure Data:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1818
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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

af:	Acentric Factor
affp:	Proton affinity
basg:	Gas basicity
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
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
rhol:	Liquid Density
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
srf:	Surface Tension
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
tt:	Triple Point Temperature
vc:	Critical Volume