Ethanethiol

Other names:	1-Ethylthiol
	1-Mercaptoethane
	Aethanethiol
	Aethylmercaptan
	C2H5SH
	Etantiolo
	Ethaanthiol
	Ethyl hydrosulfide
	Ethyl mercaptan
	Ethyl sulfhydrate
	Ethyl thioalcohol
	Ethylmercaptaan
	Ethylmerkaptan
	Etilmercaptano
	LPG ethyl mercaptan 1010
	Mercaptoethane
	NSC 93877
	Thioethanol
	Thioethyl alcohol
	UN 2363
Inchi:	InChI=1S/C2H6S/c1-2-3/h3H,2H2,1H3
InchiKey:	DNJIEGIFACGWOD-UHFFFAOYSA-N
Formula:	C2H6S
SMILES:	CCS
Mol. weight [g/mol]:	62.13
CAS:	75-08-1

Physical Properties

Property code	Value	Unit	Source
af	0.1910		KDB
affp	789.60	kJ/mol	NIST Webbook
basg	758.40	kJ/mol	NIST Webbook
chl	-2164.00	kJ/mol	NIST Webbook
chl	-2173.20 ± 0.42	kJ/mol	NIST Webbook
dm	1.50	debye	KDB
gf	-4.67	kJ/mol	KDB
hf	-46.14	kJ/mol	KDB

hf	-46.15	kJ/mol	NIST Webbook
hfl	-73.68	kJ/mol	NIST Webbook
hfus	4.98	kJ/mol	Joback Method
hvap	27.30	kJ/mol	NIST Webbook
hvap	27.50	kJ/mol	NIST Webbook
hvap	27.50	kJ/mol	NIST Webbook
hvap	27.30 ± 0.08	kJ/mol	NIST Webbook
hvap	27.52	kJ/mol	NIST Webbook
ie	9.30 ± 0.10	eV	NIST Webbook
ie	9.29 ± 0.01	eV	NIST Webbook
ie	9.31 ± 0.03	eV	NIST Webbook
ie	9.29	eV	NIST Webbook
ie	8.69	eV	NIST Webbook
ie	9.36	eV	NIST Webbook
ie	9.30	eV	NIST Webbook
ie	9.28	eV	NIST Webbook
log10ws	-0.60		Estimated Solubility Method
log10ws	-0.60		Aqueous Solubility Prediction Method
logp	0.936		Crippen Method
mcvol	55.390	ml/mol	McGowan Method
pc	5490.00 ± 50.66	kPa	NIST Webbook
pc	5490.00	kPa	KDB
rhoc	299.61 ± 1.86	kg/m3	NIST Webbook
rinpol	505.00		NIST Webbook
rinpol	528.50		NIST Webbook
rinpol	517.40		NIST Webbook
rinpol	514.20		NIST Webbook
rinpol	517.00		NIST Webbook
rinpol	482.00		NIST Webbook
rinpol	484.00		NIST Webbook
rinpol	512.60		NIST Webbook
rinpol	500.00		NIST Webbook
rinpol	517.00		NIST Webbook
rinpol	513.00		NIST Webbook
rinpol	517.00		NIST Webbook
rinpol	514.00		NIST Webbook
rinpol	520.00		NIST Webbook
rinpol	502.00		NIST Webbook
rinpol	482.00		NIST Webbook
rinpol	490.00		NIST Webbook
rinpol	500.00		NIST Webbook
rinpol	501.00		NIST Webbook
rinpol	500.00		NIST Webbook

rinpol	500.00		NIST Webbook
rinpol	496.00		NIST Webbook
rinpol	502.00		NIST Webbook
rinpol	502.00		NIST Webbook
rinpol	496.00		NIST Webbook
ripol	731.00		NIST Webbook
ripol	753.00		NIST Webbook
ripol	753.00		NIST Webbook
sl	207.02	J/mol×K	NIST Webbook
tb	308.20	K	KDB
tc	499.00	K	KDB
tc	498.70 ± 0.40	K	NIST Webbook
tc	498.80 ± 0.40	K	NIST Webbook
tc	499.00	K	NIST Webbook
tf	125.26	K	KDB
tf	126.08 ± 0.10	K	NIST Webbook
tf	125.90 ± 0.40	K	NIST Webbook
tf	126.15 ± 0.60	K	NIST Webbook
tf	125.22	K	Aqueous Solubility Prediction Method
tf	125.90 ± 0.50	K	NIST Webbook
tt	125.26 ± 0.02	K	NIST Webbook
tt	125.25 ± 0.02	K	NIST Webbook
vc	0.207	m3/kmol	KDB
zc	0.2739080		KDB
zra	0.27		KDB

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	74.41	J/mol×K	308.02	Joback Method
cpg	79.41	J/mol×K	339.82	Joback Method
cpg	84.23	J/mol×K	371.61	Joback Method
cpg	88.88	J/mol×K	403.41	Joback Method
cpg	93.35	J/mol×K	435.20	Joback Method
cpg	97.65	J/mol×K	467.00	Joback Method
cpg	101.79	J/mol×K	498.79	Joback Method
cpl	117.99	J/mol×K	299.05	NIST Webbook
hfust	4.97	kJ/mol	195.26	NIST Webbook
hfust	4.97	kJ/mol	195.30	NIST Webbook
hfust	4.97	kJ/mol	195.30	NIST Webbook

hvapt	28.40	kJ/mol	306.00	NIST Webbook
hvapt	26.78	kJ/mol	308.70	KDB
hvapt	28.40	kJ/mol	293.00	NIST Webbook
hvapt	27.50	kJ/mol	339.00	NIST Webbook
hvapt	26.30	kJ/mol	356.50	NIST Webbook
hvapt	26.60	kJ/mol	470.50	NIST Webbook
hvapt	28.40	kJ/mol	306.00	NIST Webbook
hvapt	26.79	kJ/mol	308.20	NIST Webbook
hvapt	28.70	kJ/mol	306.00	NIST Webbook
pvap	25.00	kPa	272.94	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	59.00	kPa	293.36	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	121.00	kPa	313.41	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)
rhol	839.00	kg/m3	293.00	KDB
sfust	25.48	J/mol×K	195.26	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.43813e+01
Coeff. B	-2.74888e+03
Coeff. C	-2.74390e+01
Temperature range (K), min.	222.48
Temperature range (K), max.	499.15

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	6.28903e+01
Coeff. B	-5.16282e+03
Coeff. C	-7.36756e+00
Coeff. D	7.37708e-06
Temperature range (K), min.	125.26
Temperature range (K), max.	499.15

Sources

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
KDB:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1813
KDB Vapor Pressure Data:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1813
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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
Estimated Solubility Method:	http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C75081&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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
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
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