Ethanethioamide

Other names:	Acetamide, thio-
	Acetimidic acid, thio-
	Acetothioamide
	Thiacetamide
	Thioacetamide
	TAA
	CH3CSNH2
	USAF CB-21
	USAF EK-1719
	Rcra waste number U218
	NSC 2120
Inchi:	InChI=1S/C2H5NS/c1-2(3)4/h1H3,(H2,3,4)
InchiKey:	YUKQRDCYNOVPGJ-UHFFFAOYSA-N
Formula:	C2H5NS
SMILES:	CC(N)=S
Mol. weight [g/mol]:	75.13
CAS:	62-55-5

Physical Properties

Property code	Value	Unit	Source
affp	884.60	kJ/mol	NIST Webbook
basg	852.80	kJ/mol	NIST Webbook
chs	-2030.56 ± 0.36	kJ/mol	NIST Webbook
chs	-2033.40 ± 1.10	kJ/mol	NIST Webbook
gf	149.47	kJ/mol	Joback Method
hf	12.70 ± 1.20	kJ/mol	NIST Webbook
hf	9.80 ± 0.50	kJ/mol	NIST Webbook
hfs	-73.01 ± 0.43	kJ/mol	NIST Webbook
hfs	-70.60 ± 1.10	kJ/mol	NIST Webbook
hfus	10.74	kJ/mol	Joback Method
hsub	83.30 ± 0.30	kJ/mol	NIST Webbook
hsub	82.80 ± 0.25	kJ/mol	NIST Webbook
hsub	82.80 ± 0.30	kJ/mol	NIST Webbook
hsub	83.26 ± 0.34	kJ/mol	NIST Webbook
hvap	37.42	kJ/mol	Joback Method
ie	8.36	eV	NIST Webbook
ie	8.36	eV	NIST Webbook

ie	8.35 ± 0.02	eV	NIST Webbook
ie	8.33	eV	NIST Webbook
log10ws	-0.95		Crippen Method
logp	0.292		Crippen Method
mcvol	61.070	ml/mol	McGowan Method
pc	6288.83	kPa	Joback Method
tb	387.73	K	Joback Method
tc	605.84	K	Joback Method
tf	386.42 ± 0.20	K	NIST Webbook
vc	0.212	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	97.26	J/mol×K	387.73	Joback Method
cpg	102.77	J/mol×K	424.08	Joback Method
cpg	107.82	J/mol×K	460.43	Joback Method
cpg	112.45	J/mol×K	496.79	Joback Method
cpg	116.69	J/mol×K	533.14	Joback Method
cpg	120.58	J/mol×K	569.49	Joback Method
cpg	124.17	J/mol×K	605.84	Joback Method
cps	100.30	J/mol×K	298.00	NIST Webbook
hfust	18.36	kJ/mol	385.70	NIST Webbook
hfust	18.36	kJ/mol	385.70	NIST Webbook
hsubt	82.80	kJ/mol	298.15	NIST Webbook
ssubt	277.70	J/mol×K	298.15	NIST Webbook

Sources

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C62555&Units=SI

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

Legend

affp:	Proton affinity
basg:	Gas basicity
chs:	Standard solid enthalpy of combustion
cpg:	Ideal gas heat capacity
cps:	Solid phase heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfs:	Solid phase enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hfust:	Enthalpy of fusion at a given temperature
hsub:	Enthalpy of sublimation at standard conditions
hsubt:	Enthalpy of sublimation at a given temperature
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
ssubt:	Entropy of sublimation at a given temperature
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume