Ethanol, 2-mercapto-

Other names:	1-Ethanol-2-thiol
	1-Hydroxy-2-mercaptoethane
	1-Mercapto-2-hydroxyethane
	2-Hydroxy-1-ethanethiol
	2-Hydroxyethanethiol
	2-Hydroxyethyl mercaptan
	2-ME
	2-MERCAPTOETHANOL
	2-Mercapto-1-ethanol
	2-Mercaptoethyl alcohol
	2-Thioethanol
	BETA-HYDROXYETHANETHIOL
	Emery 5791
	Ethylene glycol, monothio-
	Hydroxyethyl mercaptan
	Mercaptoethanol
	Monothioethylene glycol
	Monothioglycol
	NSC 3723
	THIOETHYLENE GLYCOL
	Thioglycol
	Thiomonoglycol
	UN 2966
	USAF EK-4196
	«beta»-Hydroxyethanethiol
	«beta»-Hydroxyethylmercaptan
	«beta»-Mercaptoethanol
	Â«betaÂ»-Hydroxyethanethiol
	Â«betaÂ»-Hydroxyethylmercaptan
	Â«betaÂ»-Mercaptoethanol
Inchi:	InChI=1S/C2H6OS/c3-1-2-4/h3-4H,1-2H2
InchiKey:	DGVVWUTYPXICAM-UHFFFAOYSA-N
Formula:	C2H6OS
SMILES:	OCCS
Mol. weight [g/mol]:	78.13
CAS:	60-24-2

Physical Properties

Property code	Value	Unit	Source
gf	-141.47	kJ/mol	Joback Method
hf	-198.36	kJ/mol	Joback Method
hfus	9.07	kJ/mol	Joback Method
hvap	43.46	kJ/mol	Joback Method
ie	9.65	eV	NIST Webbook
ie	9.10	eV	NIST Webbook
log10ws	4.71e-03		Crippen Method
logp	-0.092		Crippen Method
mcvol	61.260	ml/mol	McGowan Method
pc	6359.24	kPa	Joback Method
rinpol	717.00		NIST Webbook
rinpol	724.00		NIST Webbook
rinpol	724.00		NIST Webbook
rinpol	717.00		NIST Webbook
rinpol	725.00		NIST Webbook
rinpol	722.00		NIST Webbook
ripol	1498.00		NIST Webbook
ripol	1501.00		NIST Webbook
ripol	1498.00		NIST Webbook
ripol	1498.00		NIST Webbook
ripol	1501.00		NIST Webbook
ripol	1538.00		NIST Webbook
tb	430.20	K	NIST Webbook
tb	430.05	K	NIST Webbook
tc	587.02	K	Joback Method
tf	209.58	K	Joback Method
vc	0.221	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	125.29	J/mol×K	555.88	Joback Method
cpg	103.07	J/mol×K	400.20	Joback Method
cpg	107.90	J/mol×K	431.34	Joback Method
cpg	112.53	J/mol×K	462.47	Joback Method
cpg	116.96	J/mol×K	493.61	Joback Method

cpg	121.22	J/mol×K	524.75	Joback Method
cpg	129.18	J/mol×K	587.02	Joback Method
hvapt	54.10	kJ/mol	366.50	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	430.70	K	98.90	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.51420e+01
Coeff. B	-3.73991e+03
Coeff. C	-7.48200e+01
Temperature range (K), min.	326.59
Temperature range (K), max.	456.19

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	1.59021e+02
Coeff. B	-1.21287e+04
Coeff. C	-2.12966e+01
Coeff. D	1.57448e-05
Temperature range (K), min.	293.15
Temperature range (K), max.	440.15

Sources

KDB Vapor Pressure Data: https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1860

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
KDB:	https://www.cheric.org/files/research/kdb/mol/mol1860.mol
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C60242&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

Legend

cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
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
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume