1,2-Ethanedithiol

Other names:	1,2-Dimercaptoethane
	1,2-Dithiolethane
	1,2-Ethanethiol
	DITHIOGLYCOL
	Dithioethyleneglycol
	ETHYLENEDITHIOL
	Ethane-1,2-dithiol
	Ethylene dithioglycol
	Ethylene glycol, dithio-
	Ethylenedimercaptan
	NSC 60481
	S-ETHYLENE DIMERCAPTAN
Inchi:	InChI=1S/C2H6S2/c3-1-2-4/h3-4H,1-2H2
InchiKey:	VYMPLPIFKRHAAC-UHFFFAOYSA-N
Formula:	C2H6S2
SMILES:	SCCS
Mol. weight [g/mol]:	94.20
CAS:	540-63-6

Physical Properties

Property code	Value	Unit	Source
chl	-2794.90 ± 0.92	kJ/mol	NIST Webbook
gf	24.74	kJ/mol	Joback Method
hf	-9.30 ± 1.10	kJ/mol	NIST Webbook
hfl	-54.00 ± 1.10	kJ/mol	NIST Webbook
hfus	9.02	kJ/mol	Joback Method
hvap	44.69	kJ/mol	NIST Webbook
hvap	44.70	kJ/mol	NIST Webbook
hvap	44.70	kJ/mol	NIST Webbook
hvap	44.70 ± 0.10	kJ/mol	NIST Webbook
ie	9.30	eV	NIST Webbook
ie	9.00	eV	NIST Webbook
ie	9.35	eV	NIST Webbook
log10ws	-0.80		Crippen Method
logp	0.846		Crippen Method
mcvol	71.740	ml/mol	McGowan Method
pc	6084.49	kPa	Joback Method

rinpol	844.00		NIST Webbook
rinpol	844.00		NIST Webbook
rinpol	815.00		NIST Webbook
rinpol	805.00		NIST Webbook
rinpol	844.00		NIST Webbook
rinpol	815.00		NIST Webbook
rinpol	805.00		NIST Webbook
rinpol	801.00		NIST Webbook
ripol	1348.00		NIST Webbook
ripol	1318.00		NIST Webbook
ripol	1344.00		NIST Webbook
ripol	1330.00		NIST Webbook
ripol	1348.00		NIST Webbook
ripol	1344.00		NIST Webbook
ripol	1330.00		NIST Webbook
tb	418.00 ± 4.00	K	NIST Webbook
tb	419.20	K	NIST Webbook
tb	419.20	K	NIST Webbook
tc	593.86	K	Joback Method
tf	185.22	K	Joback Method
vc	0.256	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	106.34	J/mol×K	370.88	Joback Method
cpg	112.22	J/mol×K	408.04	Joback Method
cpg	117.81	J/mol×K	445.21	Joback Method
cpg	123.14	J/mol×K	482.37	Joback Method
cpg	128.21	J/mol×K	519.53	Joback Method
cpg	133.02	J/mol×K	556.70	Joback Method
cpg	137.57	J/mol×K	593.86	Joback Method
hvapt	37.93	kJ/mol	419.20	NIST Webbook
rfi	1.55620		293.10	Isothermal Binary Vapor-Liquid Equilibrium for 2-Methylpropane and n-Butane with 1,2-Ethanedithiol and 2-Methyl-2-propanethiol

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.44126e+01
Coeff. B	-3.54074e+03
Coeff. C	-5.76880e+01
Temperature range (K), min.	308.36
Temperature range (K), max.	446.73

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	1.27543e+02
Coeff. B	-1.00178e+04
Coeff. C	-1.67433e+01
Coeff. D	1.20163e-05
Temperature range (K), min.	328.15
Temperature range (K), max.	408.15

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
Isothermal Binary Vapor-Liquid Equilibrium for 2-Methylpropane and n-Butane with 1,2-Ethanedithiol and 2-Methyl-2-propanethiol:	https://www.doi.org/10.1021/je9003417
KDB Vapor Pressure Data:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1815
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
KDB:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1815
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C540636&Units=SI

Legend

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
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
rfi:	Refractive Index
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume