Ethene, ethoxy-

Other names:	((Vinyl)oxy)ethane
	1-Ethoxyethene
	1-Ethoxyethylene
	CH2=CHOC2H5
	ETHOXYETHENE
	EVE
	Ether, ethyl vinyl
	Ether, vinyl ethyl
	Ethoxyethylene
	Ethyl ethenyl ether
	Ethyl vinyl ether
	Ethyloxyethene
	NSC 8405
	VINYL ETHYL ETHER
	Vinamar
Inchi:	InChI=1S/C4H8O/c1-3-5-4-2/h3H,1,4H2,2H3
InchiKey:	FJKIXWOMBXYWOQ-UHFFFAOYSA-N
Formula:	C4H8O
SMILES:	C=COCC
Mol. weight [g/mol]:	72.11
CAS:	109-92-2

Physical Properties

Property code	Value	Unit	Source
af	0.2680		KDB
affp	870.10	kJ/mol	NIST Webbook
basg	840.40	kJ/mol	NIST Webbook
chg	-2577.30 ± 0.92	kJ/mol	NIST Webbook
chl	-2540.00 ± 10.00	kJ/mol	NIST Webbook
dm	1.30	debye	KDB
gf	-34.36	kJ/mol	Joback Method
hf	-140.30	kJ/mol	KDB
hf	-140.20 ± 0.96	kJ/mol	NIST Webbook
hf	-141.30 ± 0.92	kJ/mol	NIST Webbook
hf	-140.10 ± 0.96	kJ/mol	NIST Webbook
hfl	-167.90 ± 1.60	kJ/mol	NIST Webbook
hfl	-166.60 ± 1.60	kJ/mol	NIST Webbook

hfus	6.02	kJ/mol	Joback Method
hvap	26.40	kJ/mol	NIST Webbook
hvap	26.60	kJ/mol	NIST Webbook
hvap	26.60 ± 1.30	kJ/mol	NIST Webbook
ie	8.98	eV	NIST Webbook
log10ws	-0.85		Estimated Solubility Method
log10ws	-0.85		Aqueous Solubility Prediction Method
logp	1.166		Crippen Method
mcvol	68.790	ml/mol	McGowan Method
nfpaf	%!d(float64=4)		KDB
nfpah	%!d(float64=2)		KDB
nfpas	%!d(float64=2)		KDB
pc	4074.79 ± 68.94	kPa	NIST Webbook
pc	4070.00	kPa	KDB
rinpol	495.00		NIST Webbook
rinpol	499.00		NIST Webbook
rinpol	477.00		NIST Webbook
rinpol	475.00		NIST Webbook
rinpol	484.00		NIST Webbook
rinpol	495.00		NIST Webbook
rinpol	475.00		NIST Webbook
ripol	677.00		NIST Webbook
tb	308.70	K	KDB
tc	475.00 ± 2.00	K	NIST Webbook
tc	475.00	K	KDB
tf	157.35 ± 0.30	K	NIST Webbook
tf	157.85	K	NIST Webbook
tf	157.88	K	Aqueous Solubility Prediction Method
tf	157.30	K	KDB
vc	0.259	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	135.37	J/mol×K	449.17	Joback Method
cpg	141.00	J/mol×K	477.00	Joback Method
cpg	104.77	J/mol×K	310.02	Joback Method
cpg	111.22	J/mol×K	337.85	Joback Method
cpg	117.51	J/mol×K	365.68	Joback Method

cpg	123.63	J/mol×K	393.51	Joback Method
cpg	129.59	J/mol×K	421.34	Joback Method
dvisc	0.0001825	Pa×s	310.02	Joback Method
dvisc	0.0002268	Pa×s	284.24	Joback Method
dvisc	0.0019925	Pa×s	155.31	Joback Method
dvisc	0.0010073	Pa×s	181.09	Joback Method
dvisc	0.0006037	Pa×s	206.88	Joback Method
dvisc	0.0004052	Pa×s	232.66	Joback Method
dvisc	0.0002945	Pa×s	258.45	Joback Method
hvapt	29.50	kJ/mol	266.00	NIST Webbook
rhol	793.00	kg/m3	293.00	KDB

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.45277e+01
Coeff. B	-2.73192e+03
Coeff. C	-3.23100e+01
Temperature range (K), min.	224.16
Temperature range (K), max.	328.73

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	6.21960e+01
Coeff. B	-5.23422e+03
Coeff. C	-7.19624e+00
Coeff. D	6.50526e-06
Temperature range (K), min.	157.35
Temperature range (K), max.	475.15

Sources

KDB: https://www.cheric.org/files/research/kdb/mol/mol1000.mol

Estimated Solubility Method: http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt

The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C109922&Units=SI
Henry s Law Constants of Organic Compounds in Water and n-Octane at T = 298.2 K:	https://www.doi.org/10.1021/je900711h
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
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=1000
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

af:	Acentric Factor
affp:	Proton affinity
basg:	Gas basicity
chg:	Standard gas enthalpy of combustion
chl:	Standard liquid enthalpy of combustion
cpg:	Ideal gas heat capacity
dm:	Dipole Moment
dvisc:	Dynamic viscosity
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
nfpaf:	NFPA Fire Rating
nfpah:	NFPA Health Rating
nfpas:	NFPA Safety Rating
pc:	Critical Pressure
pvap:	Vapor pressure
rhol:	Liquid Density
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