Ethane, methoxy-

Other names:	C2H5OCH3
	ETHOXY METHANE
	ETHYL METHYL ETHER
	Ether, ethyl methyl
	METHOXYETHANE
	Methane, ethoxy-
	Methyl ethyl ether
	UN 1039
Inchi:	InChI=1S/C3H8O/c1-3-4-2/h3H2,1-2H3
InchiKey:	XOBKSJJDNFUZPF-UHFFFAOYSA-N
Formula:	C3H8O
SMILES:	CCOC
Mol. weight [g/mol]:	60.09
CAS:	540-67-0

Physical Properties

Property code	Value	Unit	Source
af	0.2440		KDB
affp	808.60	kJ/mol	NIST Webbook
basg	781.20	kJ/mol	NIST Webbook
chg	-2107.40 ± 0.63	kJ/mol	NIST Webbook
dm	1.20	debye	KDB
gf	-117.70	kJ/mol	KDB
hf	-216.40 ± 0.67	kJ/mol	NIST Webbook
hf	-216.60	kJ/mol	KDB
hfus	4.71	kJ/mol	Joback Method
hvap	24.68	kJ/mol	Joback Method
ie	9.60 ± 0.10	eV	NIST Webbook
ie	9.81	eV	NIST Webbook
ie	9.50	eV	NIST Webbook
ie	9.72	eV	NIST Webbook
ie	9.86	eV	NIST Webbook
ie	9.72 ± 0.07	eV	NIST Webbook
ie	9.72	eV	NIST Webbook
ie	9.72 ± 0.07	eV	NIST Webbook
log10ws	-0.17		Crippen Method
logp	0.653		Crippen Method

mcvol	59.000	ml/mol	McGowan Method
nfpaf	%!d(float64=4)		KDB
nfpah	%!d(float64=2)		KDB
pc	4400.00 ± 40.53	kPa	NIST Webbook
pc	4688.00 ± 303.98	kPa	NIST Webbook
pc	4361.00 ± 50.66	kPa	NIST Webbook
pc	4400.00	kPa	KDB
rhoc	307.03 ± 19.83	kg/m3	NIST Webbook
rhoc	272.17 ± 1.80	kg/m3	NIST Webbook
rinpol	421.00		NIST Webbook
rinpol	421.00		NIST Webbook
rinpol	419.00		NIST Webbook
rinpol	421.00		NIST Webbook
tb	312.10 ± 0.40	K	NIST Webbook
tb	283.20	K	NIST Webbook
tb	279.75 ± 0.60	K	NIST Webbook
tb	280.60	K	KDB
tc	437.80 ± 0.30	K	NIST Webbook
tc	438.03 ± 1.00	K	NIST Webbook
tc	437.80	K	KDB
tc	440.90 ± 3.00	K	NIST Webbook
tc	441.60 ± 4.00	K	NIST Webbook
tc	437.90 ± 0.30	K	NIST Webbook
tf	160.00	K	KDB
vc	0.222 ± 0.003	m3/kmol	NIST Webbook
vc	0.221	m3/kmol	KDB
zc	0.2671360		KDB

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	119.18	J/mol×K	452.73	Joback Method
cpg	88.06	J/mol×K	290.46	Joback Method
cpg	93.47	J/mol×K	317.50	Joback Method
cpg	98.79	J/mol×K	344.55	Joback Method
cpg	104.03	J/mol×K	371.59	Joback Method
cpg	109.18	J/mol×K	398.64	Joback Method
cpg	114.23	J/mol×K	425.68	Joback Method
dvisc	0.0001721	Pa×s	290.46	Joback Method
dvisc	0.0019793	Pa×s	145.80	Joback Method
dvisc	0.0009870	Pa×s	169.91	Joback Method

dvisc	0.0005850	Pa×s	194.02	Joback Method
dvisc	0.0003893	Pa×s	218.13	Joback Method
dvisc	0.0002809	Pa×s	242.24	Joback Method
dvisc	0.0002151	Pa×s	266.35	Joback Method
hvapt	26.30	kJ/mol	231.00	NIST Webbook
hvapt	24.69	kJ/mol	280.80	KDB
hvapt	30.10	kJ/mol	357.00	NIST Webbook
hvapt	37.00	kJ/mol	257.50	NIST Webbook
hvapt	37.10	kJ/mol	359.50	NIST Webbook
rhol	700.00	kg/m3	293.00	KDB
srf	0.02	N/m	298.20	KDB

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.23480e+01
Coeff. B	-1.40486e+03
Coeff. C	-1.01451e+02
Temperature range (K), min.	217.94
Temperature range (K), max.	437.80

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	2.43488e+02
Coeff. B	-1.12818e+04
Coeff. C	-3.58975e+01
Coeff. D	4.71928e-05
Temperature range (K), min.	160.00
Temperature range (K), max.	437.80

Sources

Joback Method: https://en.wikipedia.org/wiki/Joback_method

KDB: https://www.cheric.org/files/research/kdb/mol/mol998.mol

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C540670&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
KDB Vapor Pressure Data:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=998
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

af:	Acentric Factor
affp:	Proton affinity
basg:	Gas basicity
chg:	Standard gas 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
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
pc:	Critical Pressure
pvap:	Vapor pressure
rhoc:	Critical density
rhol:	Liquid Density
rinpol:	Non-polar retention indices
srf:	Surface Tension
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume
zc:	Critical Compressibility