Ethane, 1,1-diethoxy-

Other names:	1,1-DIETHOXYETHANE
	1,1-Diaethoxy-aethan
	1,1-Diethoxy-ethaan
	1,1-Dietossietano
	4-methyl-3,5-dioxaheptane
	Acetal
	Acetal diethylique
	Acetaldehyde, diethyl acetal
	Acetale
	Acetol
	CH3CH(OC2H5)2
	Capsicum annuum l
	DIETHYLACETAL
	Diaethylacetal
	Diethoxy-1,1-ethane
	Diethyl acetal
	ETHYLIDENE DIETHYL ETHER
	Ethanal diethyl acetal
	Ethylidine diethyl ether
	NSC 7624
	UN 1088
	USAF DO-45
	acetal (acetaldehyde diethyl acetal)
	acetaldehyde diethyl acetal
Inchi:	InChI=1S/C6H14O2/c1-4-7-6(3)8-5-2/h6H,4-5H2,1-3H3
InchiKey:	DHKHKXVYLBGOIT-UHFFFAOYSA-N
Formula:	C6H14O2
SMILES:	CCOC(C)OCC
Mol. weight [g/mol]:	118.17
CAS:	105-57-7

Physical Properties

Property code	Value	Unit	Source
chl	-3870.50 ± 2.30	kJ/mol	NIST Webbook
gf	-212.80	kJ/mol	Joback Method
hf	-453.60 ± 3.10	kJ/mol	NIST Webbook

hfus	10.15	kJ/mol	Joback Method
hvap	39.60 ± 0.30	kJ/mol	NIST Webbook
hvap	37.80 ± 0.84	kJ/mol	NIST Webbook
ie	9.20	eV	NIST Webbook
ie	9.78	eV	NIST Webbook
log10ws	-0.43		Estimated Solubility Method
log10ws	-0.43		Aqueous Solubility Prediction Method
logp	1.405		Crippen Method
mcvol	107.140	ml/mol	McGowan Method
nfpaf	%!d(float64=3)		KDB
nfpah	%!d(float64=2)		KDB
pc	3220.00 ± 20.00	kPa	NIST Webbook
rinpol	726.00		NIST Webbook
rinpol	725.10		NIST Webbook
rinpol	734.00		NIST Webbook
rinpol	710.00		NIST Webbook
rinpol	726.00		NIST Webbook
rinpol	727.00		NIST Webbook
rinpol	743.00		NIST Webbook
rinpol	726.00		NIST Webbook
rinpol	727.00		NIST Webbook
rinpol	715.00		NIST Webbook
rinpol	718.00		NIST Webbook
rinpol	730.00		NIST Webbook
rinpol	725.00		NIST Webbook
rinpol	722.16		NIST Webbook
rinpol	727.00		NIST Webbook
rinpol	719.00		NIST Webbook
rinpol	726.00		NIST Webbook
rinpol	730.00		NIST Webbook
rinpol	719.00		NIST Webbook
rinpol	726.00		NIST Webbook
rinpol	719.00		NIST Webbook
rinpol	726.00		NIST Webbook
rinpol	714.00		NIST Webbook
rinpol	725.00		NIST Webbook
rinpol	736.00		NIST Webbook
rinpol	729.00		NIST Webbook
rinpol	724.00		NIST Webbook
rinpol	730.00		NIST Webbook
rinpol	730.00		NIST Webbook
rinpol	730.00		NIST Webbook
rinpol	717.00		NIST Webbook

rinpol	717.30	NIST Webbook
rinpol	710.00	NIST Webbook
rinpol	725.00	NIST Webbook
rinpol	719.00	NIST Webbook
rinpol	725.00	NIST Webbook
rinpol	722.16	NIST Webbook
rinpol	727.00	NIST Webbook
rinpol	726.00	NIST Webbook
rinpol	715.00	NIST Webbook
rinpol	734.00	NIST Webbook
rinpol	730.00	NIST Webbook
rinpol	717.30	NIST Webbook
rinpol	720.00	NIST Webbook
rinpol	717.00	NIST Webbook
rinpol	710.00	NIST Webbook
rinpol	729.00	NIST Webbook
ripol	900.00	NIST Webbook
ripol	890.00	NIST Webbook
ripol	866.00	NIST Webbook
ripol	867.00	NIST Webbook
ripol	886.00	NIST Webbook
ripol	900.00	NIST Webbook
ripol	866.00	NIST Webbook
ripol	890.00	NIST Webbook
ripol	889.00	NIST Webbook
ripol	928.00	NIST Webbook
ripol	886.00	NIST Webbook
ripol	910.00	NIST Webbook
ripol	900.00	NIST Webbook
ripol	900.00	NIST Webbook
ripol	880.00	NIST Webbook
ripol	930.00	NIST Webbook
ripol	925.00	NIST Webbook
ripol	880.00	NIST Webbook
ripol	890.00	NIST Webbook
ripol	890.00	NIST Webbook
ripol	889.00	NIST Webbook
ripol	890.00	NIST Webbook
ripol	898.00	NIST Webbook
ripol	900.00	NIST Webbook
ripol	889.00	NIST Webbook
ripol	891.00	NIST Webbook
ripol	892.00	NIST Webbook
ripol	889.00	NIST Webbook

ripol	894.00		NIST Webbook
ripol	928.00		NIST Webbook
ripol	925.00		NIST Webbook
ripol	910.00		NIST Webbook
tb	376.00	K	NIST Webbook
tb	375.20	K	NIST Webbook
tb	376.40	K	NIST Webbook
tb	376.00 ± 2.00	K	NIST Webbook
tb	376.40 ± 1.50	K	NIST Webbook
tb	375.35 ± 1.50	K	NIST Webbook
tb	375.40	K	KDB
tb	355.75 ± 0.50	K	NIST Webbook
tb	376.70 ± 0.50	K	NIST Webbook
tc	539.70 ± 0.50	K	NIST Webbook
tc	527.00	K	KDB
tc	527.60 ± 10.00	K	NIST Webbook
tf	173.00	K	KDB
vc	0.402	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	204.59	J/mol×K	381.08	Joback Method
cpg	214.84	J/mol×K	409.27	Joback Method
cpg	224.86	J/mol×K	437.45	Joback Method
cpg	234.65	J/mol×K	465.64	Joback Method
cpg	244.19	J/mol×K	493.83	Joback Method
cpg	253.48	J/mol×K	522.01	Joback Method
cpg	262.51	J/mol×K	550.20	Joback Method
cpl	237.70	J/mol×K	298.00	NIST Webbook
dvisc	0.0018547	Pa×s	219.21	Joback Method
dvisc	0.0046299	Pa×s	186.84	Joback Method
dvisc	0.0009402	Pa×s	251.59	Joback Method
dvisc	0.0005565	Pa×s	283.96	Joback Method
dvisc	0.0003667	Pa×s	316.33	Joback Method
dvisc	0.0002611	Pa×s	348.71	Joback Method
dvisc	0.0001969	Pa×s	381.08	Joback Method
hfust	10.95	kJ/mol	167.00	NIST Webbook
hvapt	41.60	kJ/mol	332.50	NIST Webbook
hvapt	36.20	kJ/mol	315.50	NIST Webbook
hvapt	39.80	kJ/mol	308.00	NIST Webbook

pvap	19.00	kPa	328.35	Vapor Liquid Equilibrium for Binary System of 2-Propanol + 1,1-Diethoxyethane at 353 K and Ethyl ethanoate + 1,1-Diethoxyethane at 348 K and 2-Propanone + 1,1-Diethoxyethane at 328 K
pvap	32.10	kPa	341.62	Vapor Liquid Equilibrium for Binary System of 2-Propanol + 1,1-Diethoxyethane at 353 K and Ethyl ethanoate + 1,1-Diethoxyethane at 348 K and 2-Propanone + 1,1-Diethoxyethane at 328 K
pvap	36.70	kPa	345.13	Vapor Liquid Equilibrium for Binary System of 2-Propanol + 1,1-Diethoxyethane at 353 K and Ethyl ethanoate + 1,1-Diethoxyethane at 348 K and 2-Propanone + 1,1-Diethoxyethane at 328 K
pvap	41.10	kPa	348.33	Vapor Liquid Equilibrium for Binary System of 2-Propanol + 1,1-Diethoxyethane at 353 K and Ethyl ethanoate + 1,1-Diethoxyethane at 348 K and 2-Propanone + 1,1-Diethoxyethane at 328 K
pvap	49.20	kPa	353.38	Vapor Liquid Equilibrium for Binary System of 2-Propanol + 1,1-Diethoxyethane at 353 K and Ethyl ethanoate + 1,1-Diethoxyethane at 348 K and 2-Propanone + 1,1-Diethoxyethane at 328 K

pvap	57.90	kPa	357.95	Vapor Liquid Equilibrium for Binary System of 2-Propanol + 1,1-Diethoxyethane at 353 K and Ethyl ethanoate + 1,1-Diethoxyethane at 348 K and 2-Propanone + 1,1-Diethoxyethane at 328 K
pvap	66.10	kPa	361.96	Vapor Liquid Equilibrium for Binary System of 2-Propanol + 1,1-Diethoxyethane at 353 K and Ethyl ethanoate + 1,1-Diethoxyethane at 348 K and 2-Propanone + 1,1-Diethoxyethane at 328 K
pvap	72.30	kPa	364.68	Vapor Liquid Equilibrium for Binary System of 2-Propanol + 1,1-Diethoxyethane at 353 K and Ethyl ethanoate + 1,1-Diethoxyethane at 348 K and 2-Propanone + 1,1-Diethoxyethane at 328 K
pvap	77.90	kPa	366.99	Vapor Liquid Equilibrium for Binary System of 2-Propanol + 1,1-Diethoxyethane at 353 K and Ethyl ethanoate + 1,1-Diethoxyethane at 348 K and 2-Propanone + 1,1-Diethoxyethane at 328 K
pvap	83.10	kPa	369.09	Vapor Liquid Equilibrium for Binary System of 2-Propanol + 1,1-Diethoxyethane at 353 K and Ethyl ethanoate + 1,1-Diethoxyethane at 348 K and 2-Propanone + 1,1-Diethoxyethane at 328 K

pvap	90.10	kPa	371.70	Vapor Liquid Equilibrium for Binary System of 2-Propanol + 1,1-Diethoxyethane at 353 K and Ethyl ethanoate + 1,1-Diethoxyethane at 348 K and 2-Propanone + 1,1-Diethoxyethane at 328 K
pvap	94.80	kPa	373.41	Vapor Liquid Equilibrium for Binary System of 2-Propanol + 1,1-Diethoxyethane at 353 K and Ethyl ethanoate + 1,1-Diethoxyethane at 348 K and 2-Propanone + 1,1-Diethoxyethane at 328 K
pvap	100.00	kPa	375.27	Vapor Liquid Equilibrium for Binary System of 2-Propanol + 1,1-Diethoxyethane at 353 K and Ethyl ethanoate + 1,1-Diethoxyethane at 348 K and 2-Propanone + 1,1-Diethoxyethane at 328 K
srf	0.02	N/m	298.15	Excess Molar Volumes and Surface Tensions of 1,2,4-Trimethylbenzene and 1,3,5-Trimethylbenzene with 1,1-Diethoxyethane and 2,2-Dimethoxypropane at (298.15, 308.15, and 313.15) K
srf	0.02	N/m	308.15	Excess Molar Volumes and Surface Tensions of 1,2,4-Trimethylbenzene and 1,3,5-Trimethylbenzene with 1,1-Diethoxyethane and 2,2-Dimethoxypropane at (298.15, 308.15, and 313.15) K

srf	0.02	N/m	313.15	Excess Molar Volumes and Surface Tensions of 1,2,4-Trimethylbenzene and 1,3,5-Trimethylbenzene with 1,1-Diethoxyethane and 2,2-Dimethoxypropane at (298.15, 308.15, and 313.15) K

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	294.20	K	2.90	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.50751e+01
Coeff. B	-3.39836e+03
Coeff. C	-5.08590e+01
Temperature range (K), min.	280.67
Temperature range (K), max.	398.92

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	8.46597e+01
Coeff. B	-7.69833e+03
Coeff. C	-1.01631e+01
Coeff. D	5.21530e-06
Temperature range (K), min.	173.15
Temperature range (K), max.	541.00

Sources

Excess Molar Enthalpies for the Binary Systems of Benzene or Cyclohexane with 1,1-Diethoxyethane at 323.15 K or with 2,2-Dimethoxybutane at 303.15 K and Infinite Dilution Activity Coefficients in 1,1-Diethoxyethane:	https://www.doi.org/10.1021/je020195l
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
Estimated Solubility Method:	http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt
KDB Vapor Pressure Data:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1051
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Excess Molar Volumes and Surface Tensions of 1,2,4- Trimethylbenzene and 1,3,5- Trimethylbenzene with 1,1-Diethoxyethane and 2,2-Dimethoxypropane at (298.15, 308.15, and 313.15) K:	https://www.doi.org/10.1021/je060490w
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C105577&Units=SI
Vapor Liquid Equilibrium for Binary System of 2-Propanol + 1,1-Diethoxyethane at 353 K and Ethyl ethanoate + 1,1-Diethoxyethane at 348 K and 2-Propanone + 1,1-Diethoxyethane at 328 K:	https://www.doi.org/10.1021/je049816w
Modified Wilson:	http://link.springer.com/article/10.1007/BF02311772
KDB:	https://www.cheric.org/files/research/kdb/mol/mol1051.mol

Legend

chl:	Standard liquid enthalpy of combustion
cpg:	Ideal gas heat capacity
cpl:	Liquid phase heat capacity
dvisc:	Dynamic viscosity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hfust:	Enthalpy of fusion at a given temperature
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
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
srf:	Surface Tension
tb:	Normal Boiling Point Temperature

tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume