Ethane, 1,1'-[methylenebis(oxy)]bis-

Other names:	1,1-diethoxymethane
	3,5-dioxaheptane
	Formaldehyde diethyl acetal
	NSC 6754
	UN 2373
	diethoxymethane
	diethyl formal
	diethylformal
	ethoxymethyl ethyl ether
	ethylal
	formaldehyde, diethyl acetal
	methane, diethoxy-
Inchi:	InChI=1S/C5H12O2/c1-3-6-5-7-4-2/h3-5H2,1-2H3
InchiKey:	KLKFAASOGCDTDT-UHFFFAOYSA-N
Formula:	C5H12O2
SMILES:	CCOCOCC
Mol. weight [g/mol]:	104.15
CAS:	462-95-3

Physical Properties

Property code	Value	Unit	Source
af	0.3802		Cheméo Relay (1.0)
chl	-3232.12 ± 0.79	kJ/mol	NIST Webbook
chl	-3233.80 ± 0.40	kJ/mol	NIST Webbook
gf	-218.78	kJ/mol	Joback Method
hf	-414.76 ± 0.86	kJ/mol	NIST Webbook
hf	-413.10	kJ/mol	NIST Webbook
hfl	-450.41 ± 0.84	kJ/mol	NIST Webbook
hfl	-448.70 ± 0.40	kJ/mol	NIST Webbook
hfus	11.08	kJ/mol	Joback Method
hvap	35.70 ± 0.20	kJ/mol	NIST Webbook
hvap	35.74	kJ/mol	NIST Webbook
hvap	35.70	kJ/mol	NIST Webbook
hvap	35.65 ± 0.17	kJ/mol	NIST Webbook
hvap	37.00 ± 2.00	kJ/mol	NIST Webbook
ie	9.70 ± 0.05	eV	NIST Webbook
log10ws	-0.41		Cheméo Relay (1.0)

logp	1.017		Crippen Method
mcvol	93.050	ml/mol	McGowan Method
pc	3333.53	kPa	Joback Method
rinpol	636.00		NIST Webbook
rinpol	635.00		NIST Webbook
rinpol	657.74		NIST Webbook
rinpol	649.00		NIST Webbook
rinpol	657.74		NIST Webbook
rinpol	647.00		NIST Webbook
tb	361.10 ± 0.60	K	NIST Webbook
tb	360.65 ± 0.50	K	NIST Webbook
tb	361.05 ± 0.30	K	NIST Webbook
tb	361.50 ± 0.60	K	NIST Webbook
tb	361.10	K	NIST Webbook
tb	362.20	K	NIST Webbook
tb	360.70	K	NIST Webbook
tc	523.60	K	Cheméo Relay (1.0)
tf	207.20 ± 1.50	K	NIST Webbook
tf	206.65 ± 0.50	K	NIST Webbook
tf	206.00 ± 2.00	K	NIST Webbook
vc	0.348	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	218.03	J/mol×K	524.09	Joback Method
cpg	202.53	J/mol×K	468.94	Joback Method
cpg	169.54	J/mol×K	358.64	Joback Method
cpg	178.02	J/mol×K	386.21	Joback Method
cpg	186.35	J/mol×K	413.79	Joback Method
cpg	194.52	J/mol×K	441.36	Joback Method
cpg	210.37	J/mol×K	496.51	Joback Method
dvisc	0.0025228	Pa×s	190.57	Joback Method
dvisc	0.0012659	Pa×s	218.58	Joback Method
dvisc	0.0007430	Pa×s	246.59	Joback Method
dvisc	0.0004861	Pa×s	274.61	Joback Method
dvisc	0.0003441	Pa×s	302.62	Joback Method
dvisc	0.0002582	Pa×s	330.63	Joback Method
dvisc	0.0002027	Pa×s	358.64	Joback Method
hvapt	31.33	kJ/mol	361.10	NIST Webbook
hvapt	36.10	kJ/mol	317.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.15689e+01
Coeff. B	-2.59148e+03
Coeff. C	-3.56060e+01
Temperature range (K), min.	265.32
Temperature range (K), max.	449.75

Sources

Measurement and thermodynamic modeling of ternary (liquid + liquid) equilibrium for extraction of ethanol from diethoxymethane solution with different solvents:	https://www.doi.org/10.1016/j.jct.2017.03.014
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C462953&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0, beta):	
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
Partial molar volumes of organic solutes in water. XVIII: Selected polyethers(aq) and 3,6-dioxa-1-heptanol(aq) at T = (298 to 573) K and at pressures up to 30 MPa:	https://www.doi.org/10.1016/j.jct.2007.01.015
Cheméo Relay (1.0):	

Legend

af:	Acentric Factor
chl:	Standard liquid enthalpy of combustion
cpg:	Ideal gas heat capacity
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
pc:	Critical Pressure
pvap:	Vapor pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume