Methane, diethoxy-

Other names:	1,1-Diethoxymethane
	3,5-Dioxaheptane
	Diethoxymethane
	Diethylformal
	Ethane, 1,1'-[methylenebis(oxy)]bis-
	Ethoxymethyl ethyl ether
	Ethylal
	Formaldehyde diethyl acetal
	NSC 6754
	UN 2373
	diethyl formal
	formaldehyde, diethyl acetal
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
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	-448.70 ± 0.40	kJ/mol	NIST Webbook
hfl	-450.41 ± 0.84	kJ/mol	NIST Webbook
hfus	11.08	kJ/mol	Joback Method
hvap	35.70 ± 0.20	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
hvap	35.74	kJ/mol	NIST Webbook
ie	9.70 ± 0.05	eV	NIST Webbook
log10ws	-0.59		Crippen Method
logp	1.017		Crippen Method

mcvol	93.050	ml/mol	McGowan Method
pc	3333.53	kPa	Joback Method
rinpol	657.74		NIST Webbook
rinpol	636.00		NIST Webbook
rinpol	635.00		NIST Webbook
rinpol	649.00		NIST Webbook
rinpol	657.74		NIST Webbook
rinpol	647.00		NIST Webbook
tb	358.64	K	Joback Method
tc	524.09	K	Joback Method
tf	206.00 ± 2.00	K	NIST Webbook
tf	207.20 ± 1.50	K	NIST Webbook
tf	206.65 ± 0.50	K	NIST Webbook
vc	0.351	m3/kmol	Joback Method

Temperature Dependent Properties

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

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C462953&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
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
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

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