1,1-Ethanediol, diacetate

Other names:	1,1'-Diacetoxy-ethane
	1,1-Diacetoxyethane
	1,1-ETHANEDIOL
	DIACETATE
	ETHYLIDENE ACETATE
	Ethylidene diacetate
	ethylidene diethanoate
Inchi:	InChI=1S/C6H10O4/c1-4(7)9-6(3)10-5(2)8/h6H,1-3H3
InchiKey:	ACKALUBLCWJVNB-UHFFFAOYSA-N
Formula:	C6H10O4
SMILES:	CC(=O)OC(C)OC(C)=O
Mol. weight [g/mol]:	146.14
CAS:	542-10-9

Physical Properties

Property code	Value	Unit	Source
chl	-2918.70 ± 1.00	kJ/mol	NIST Webbook
gf	-470.64	kJ/mol	Joback Method
hf	-812.60 ± 1.10	kJ/mol	NIST Webbook
hfl	-871.50 ± 1.00	kJ/mol	NIST Webbook
hfus	13.35	kJ/mol	Joback Method
hvap	59.00 ± 1.00	kJ/mol	NIST Webbook
hvap	58.90	kJ/mol	NIST Webbook
log10ws	-0.67		Crippen Method
logp	0.459		Crippen Method
mcvol	110.280	ml/mol	McGowan Method
pc	2970.00	kPa	Critical Point and Vapor Pressure Measurements for 17 Compounds by a Low Residence Time Flow Method
rinpol	786.00		NIST Webbook
rinpol	789.00		NIST Webbook
tb	488.82	K	Joback Method
tc	680.73	K	Joback Method
tf	286.70	K	Joback Method
vc	0.413	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	289.02	J/mol×K	680.73	Joback Method
cpg	236.68	J/mol×K	488.82	Joback Method
cpg	246.23	J/mol×K	520.80	Joback Method
cpg	255.46	J/mol×K	552.79	Joback Method
cpg	264.37	J/mol×K	584.77	Joback Method
cpg	272.95	J/mol×K	616.76	Joback Method
cpg	281.17	J/mol×K	648.74	Joback Method
dvisc	0.0002524	Pa×s	488.82	Joback Method
dvisc	0.0027257	Pa×s	286.70	Joback Method
dvisc	0.0014884	Pa×s	320.39	Joback Method
dvisc	0.0009119	Pa×s	354.07	Joback Method
dvisc	0.0006083	Pa×s	387.76	Joback Method
dvisc	0.0004330	Pa×s	421.45	Joback Method
dvisc	0.0003241	Pa×s	455.13	Joback Method
hvapt	49.70	kJ/mol	390.50	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	339.20	K	1.30	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.40900e+01
Coeff. B	-3.15761e+03
Coeff. C	-1.08775e+02
Temperature range (K), min.	337.55
Temperature range (K), max.	468.47

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	3.44052e+02
Coeff. B	-2.10841e+04
Coeff. C	-4.89250e+01
Coeff. D	3.21924e-05
Temperature range (K), min.	292.00
Temperature range (K), max.	635.00

Sources

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
KDB Vapor Pressure Data:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1178
KDB:	https://www.cheric.org/files/research/kdb/mol/mol1178.mol
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C542109&Units=SI
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
Critical Point and Vapor Pressure Measurements for 17 Compounds by a Low Residence Time Flow Method:	https://www.doi.org/10.1021/je060269j
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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