1,2-Ethanediol, diacetate

Other names:	1,2-Diacetoxyethane
	1,2-Ethanediol, 1,2-diacetate
	1,2-ethanediol, diethanoate
	2-Acetyloxyethyl acetate
	Aptex Donor H-plus
	CH3C(O)OCH2CH2OC(O)CH3
	Ethanediol diacetate
	Ethylene acetate
	Ethylene diacetate
	Ethylene diacetin
	Ethylene diethanoate
	Ethylene glycol acetate
	Ethylene glycol diacetate
	Ethylene glycol, diacetate
	Ethylene gycol diacetate
	Glycol diacetate
	NSC 8853
	ethanoic acid, 1,2-ethanediyl ester
	ethylidene diacetate
Inchi:	InChI=1S/C6H10O4/c1-5(7)9-3-4-10-6(2)8/h3-4H2,1-2H3
InchiKey:	JTXMVXSTHSMVQF-UHFFFAOYSA-N
Formula:	C6H10O4
SMILES:	CC(=O)OCCOC(C)=O
Mol. weight [g/mol]:	146.14
CAS:	111-55-7

Physical Properties

Property code	Value	Unit	Source
gf	-468.20	kJ/mol	Joback Method
hf	-656.77	kJ/mol	Joback Method
hfus	16.87	kJ/mol	Joback Method
hvap	61.44 ± 0.15	kJ/mol	NIST Webbook
hvap	61.04 ± 0.02	kJ/mol	NIST Webbook
hvap	61.40 ± 0.20	kJ/mol	NIST Webbook
hvap	61.40 ± 0.20	kJ/mol	NIST Webbook
hvap	61.00 ± 0.10	kJ/mol	NIST Webbook
log10ws	-0.06		Crippen Method

logp	0.113		Crippen Method
mcvol	110.280	ml/mol	McGowan Method
pc	3452.08	kPa	Joback Method
rinpol	1002.00		NIST Webbook
rinpol	993.90		NIST Webbook
rinpol	1010.00		NIST Webbook
rinpol	1007.00		NIST Webbook
rinpol	1008.00		NIST Webbook
rinpol	1002.00		NIST Webbook
rinpol	1006.00		NIST Webbook
rinpol	1011.00		NIST Webbook
rinpol	1007.00		NIST Webbook
rinpol	1008.00		NIST Webbook
rinpol	1009.00		NIST Webbook
rinpol	1010.00		NIST Webbook
rinpol	1007.00		NIST Webbook
rinpol	993.90		NIST Webbook
rinpol	1010.00		NIST Webbook
rinpol	1008.00		NIST Webbook
rinpol	1006.00		NIST Webbook
rinpol	1007.00		NIST Webbook
ripol	1490.00		NIST Webbook
ripol	1531.00		NIST Webbook
ripol	1555.00		NIST Webbook
ripol	1539.00		NIST Webbook
ripol	1490.00		NIST Webbook
tb	466.15 ± 1.50	K	NIST Webbook
tb	463.20	K	NIST Webbook
tb	459.70	K	NIST Webbook
tc	677.07	K	Joback Method
tf	301.70	K	Joback Method
vc	0.419	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	236.42	J/mol×K	489.26	Joback Method
cpg	245.69	J/mol×K	520.56	Joback Method
cpg	287.43	J/mol×K	677.07	Joback Method
cpg	279.74	J/mol×K	645.76	Joback Method
cpg	271.71	J/mol×K	614.46	Joback Method

cpg	263.35	J/mol×K	583.16	Joback Method
cpg	254.67	J/mol×K	551.86	Joback Method
cpl	269.20	J/mol×K	298.15	NIST Webbook
cpl	310.00	J/mol×K	298.15	NIST Webbook
dvisc	0.0008254	Pa×s	364.22	Joback Method
dvisc	0.0012506	Pa×s	332.96	Joback Method
dvisc	0.0002663	Pa×s	489.26	Joback Method
dvisc	0.0003335	Pa×s	458.00	Joback Method
dvisc	0.0004316	Pa×s	426.74	Joback Method
dvisc	0.0005818	Pa×s	395.48	Joback Method
dvisc	0.0020653	Pa×s	301.70	Joback Method
hvapt	57.60	kJ/mol	418.00	NIST Webbook
hvapt	55.20	kJ/mol	387.50	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	3.83647e+02
Coeff. B	-2.43192e+04
Coeff. C	-5.43240e+01
Coeff. D	3.22152e-05
Temperature range (K), min.	242.15
Temperature range (K), max.	653.00

Sources

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

Salt Effect on the Liquid-Liquid Equilibrium for the Water-Ethylene Glycol-Ethylene Glycol Diacetate System: https://www.doi.org/10.1021/acs.jced.8b01248

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C111557&Units=SI

KDB Vapor Pressure Data: https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1073

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Measurement of the thermodynamic properties for the reactive system ethylene glycol-acetic acid: https://www.doi.org/10.1016/j.fluid.2007.05.030

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

KDB: https://www.cheric.org/files/research/kdb/mol/mol1073.mol

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

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
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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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