1,3-Dioxolan-2-one

Other names:	1,3-Dioxacyclopentan-2-one
	2-Dioxolone
	CYCLIC ETHYLENE CARBONATE
	Carbonic acid, cyclic ethylene ester
	Dioxolone-2
	ETHYLENE CARBONATE
	ETHYLENE GLYCOL CARBONATE
	Ethylene glycol, cyclic carbonate
	Ethylenester kyseliny uhlicite
	Glycol carbonate
	NSC 11801
	Texacar EC
	carbonic acid, ethylene ester
Inchi:	InChI=1S/C3H4O3/c4-3-5-1-2-6-3/h1-2H2
InchiKey:	KMTRUDSVKNLOMY-UHFFFAOYSA-N
Formula:	C3H4O3
SMILES:	O=C1OCCO1
Mol. weight [g/mol]:	88.06
CAS:	96-49-1

Physical Properties

Property code	Value	Unit	Source
affp	814.20	kJ/mol	NIST Webbook
basg	784.40	kJ/mol	NIST Webbook
chl	-1069.30 ± 2.10	kJ/mol	NIST Webbook
chs	-1170.60 ± 0.40	kJ/mol	NIST Webbook
chs	-1165.90 ± 3.70	kJ/mol	NIST Webbook
chs	-1161.40	kJ/mol	NIST Webbook
chs	-1171.32	kJ/mol	NIST Webbook
gf	-276.19	kJ/mol	Joback Method
hf	-503.00 ± 4.20	kJ/mol	NIST Webbook
hfl	-682.80 ± 2.10	kJ/mol	NIST Webbook
hfs	-581.60 ± 0.40	kJ/mol	NIST Webbook
hfs	-586.30 ± 3.80	kJ/mol	NIST Webbook
hfs	-590.90	kJ/mol	NIST Webbook
hfus	11.86	kJ/mol	Joback Method
hvap	60.80 ± 0.10	kJ/mol	NIST Webbook

hvap	78.50 ± 4.20	kJ/mol	NIST Webbook
hvap	179.80	kJ/mol	NIST Webbook
hvap	64.00 ± 0.10	kJ/mol	NIST Webbook
hvap	63.40 ± 0.30	kJ/mol	NIST Webbook
hvap	62.40	kJ/mol	NIST Webbook
ie	10.40	eV	NIST Webbook
ie	10.40	eV	NIST Webbook
ie	11.10	eV	NIST Webbook
ie	11.47	eV	NIST Webbook
ie	10.70	eV	NIST Webbook
log10ws	0.10		Crippen Method
logp	0.153		Crippen Method
mcvol	55.580	ml/mol	McGowan Method
pc	6141.84	kPa	Joback Method
ss	132.54	J/mol×K	NIST Webbook
ss	132.54	J/mol×K	NIST Webbook
tb	409.71	K	Joback Method
tc	635.21	K	Joback Method
tf	309.45 ± 0.20	K	NIST Webbook
tf	309.50 ± 0.60	K	NIST Webbook
tf	308.53	K	Efficient determination of crystallisation and melting points at low cooling and heating rates with novel computer controlled equipment
tf	308.95 ± 0.50	K	NIST Webbook
tf	311.15 ± 1.50	K	NIST Webbook
tf	309.65 ± 0.15	K	NIST Webbook
tf	312.95 ± 0.20	K	NIST Webbook
tf	308.90 ± 0.80	K	NIST Webbook
tf	311.15	K	Characterization on the exothermic behaviors of cathode materials reacted with ethylene carbonate in lithium-ion battery studied by differential scanning calorimeter (DSC)
tt	309.49 ± 0.02	K	NIST Webbook
tt	309.49	K	KDB
tt	309.47 ± 0.00	K	NIST Webbook
vc	0.195	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	147.91	J/mol×K	635.21	Joback Method
cpg	128.08	J/mol×K	522.46	Joback Method
cpg	135.02	J/mol×K	560.05	Joback Method
cpg	141.63	J/mol×K	597.63	Joback Method
cpg	105.45	J/mol×K	409.71	Joback Method
cpg	113.28	J/mol×K	447.29	Joback Method
cpg	120.83	J/mol×K	484.88	Joback Method
cpl	157.63	J/mol×K	393.15	Vapor Pressure and Liquid Heat Capacity of Alkylene Carbonates
cpl	158.51	J/mol×K	398.15	Vapor Pressure and Liquid Heat Capacity of Alkylene Carbonates
cpl	133.90	J/mol×K	323.15	NIST Webbook
cpl	155.87	J/mol×K	383.15	Vapor Pressure and Liquid Heat Capacity of Alkylene Carbonates
cpl	156.75	J/mol×K	388.15	Vapor Pressure and Liquid Heat Capacity of Alkylene Carbonates
cps	117.44	J/mol×K	298.15	NIST Webbook
cps	117.44	J/mol×K	298.15	NIST Webbook
hfust	13.30	kJ/mol	309.50	NIST Webbook
hfust	13.29	kJ/mol	309.49	NIST Webbook
hfust	13.29	kJ/mol	309.49	NIST Webbook
hfust	13.02	kJ/mol	311.20	NIST Webbook
hfust	13.30	kJ/mol	309.50	NIST Webbook
hsubt	68.70	kJ/mol	285.00	NIST Webbook
hvapt	56.48	kJ/mol	423.00	NIST Webbook
hvapt	60.30	kJ/mol	408.50	NIST Webbook
hvapt	56.30	kJ/mol	408.50	NIST Webbook
hvapt	55.00	kJ/mol	400.50	NIST Webbook
hvapt	59.60	kJ/mol	409.00	NIST Webbook
pvap	0.02	kPa	314.50	Vapour pressure and enthalpy of vaporization of cyclic alkylene carbonates
pvap	0.47	kPa	369.50	Vapour pressure and enthalpy of vaporization of cyclic alkylene carbonates

pvap	0.04	kPa	333.15	Low pressure methane solubility in lithium-ion batteries based solvents and electrolytes as a function of temperature. Measurement and prediction	
pvap	0.07	kPa	338.15	Low pressure methane solubility in lithium-ion batteries based solvents and electrolytes as a function of temperature. Measurement and prediction	
pvap	0.09	kPa	343.15	Low pressure methane solubility in lithium-ion batteries based solvents and electrolytes as a function of temperature. Measurement and prediction	
pvap	0.01	kPa	310.30	Vapour pressure and enthalpy of vaporization of cyclic alkylene carbonates	
pvap	0.02	kPa	314.40	Vapour pressure and enthalpy of vaporization of cyclic alkylene carbonates	
pvap	0.12	kPa	348.15	Low pressure methane solubility in lithium-ion batteries based solvents and electrolytes as a function of temperature. Measurement and prediction	
pvap	0.02	kPa	317.30	Vapour pressure and enthalpy of vaporization of cyclic alkylene carbonates	

pvap	0.02	kPa	320.30	Vapour pressure and enthalpy of vaporization of cyclic alkylene carbonates
pvap	0.02	kPa	320.40	Vapour pressure and enthalpy of vaporization of cyclic alkylene carbonates
pvap	0.03	kPa	323.50	Vapour pressure and enthalpy of vaporization of cyclic alkylene carbonates
pvap	0.03	kPa	324.40	Vapour pressure and enthalpy of vaporization of cyclic alkylene carbonates
pvap	0.04	kPa	327.40	Vapour pressure and enthalpy of vaporization of cyclic alkylene carbonates
pvap	0.04	kPa	328.60	Vapour pressure and enthalpy of vaporization of cyclic alkylene carbonates
pvap	0.05	kPa	331.30	Vapour pressure and enthalpy of vaporization of cyclic alkylene carbonates
pvap	0.06	kPa	333.60	Vapour pressure and enthalpy of vaporization of cyclic alkylene carbonates
pvap	0.07	kPa	335.40	Vapour pressure and enthalpy of vaporization of cyclic alkylene carbonates
pvap	0.08	kPa	338.70	Vapour pressure and enthalpy of vaporization of cyclic alkylene carbonates
pvap	0.10	kPa	341.40	Vapour pressure and enthalpy of vaporization of cyclic alkylene carbonates
pvap	0.10	kPa	342.30	Vapour pressure and enthalpy of vaporization of cyclic alkylene carbonates

pvap	0.11	kPa	343.80	Vapour pressure and enthalpy of vaporization of cyclic alkylene carbonates
pvap	0.12	kPa	345.20	Vapour pressure and enthalpy of vaporization of cyclic alkylene carbonates
pvap	0.14	kPa	347.60	Vapour pressure and enthalpy of vaporization of cyclic alkylene carbonates
pvap	0.15	kPa	349.00	Vapour pressure and enthalpy of vaporization of cyclic alkylene carbonates
pvap	0.19	kPa	352.40	Vapour pressure and enthalpy of vaporization of cyclic alkylene carbonates
pvap	0.20	kPa	354.00	Vapour pressure and enthalpy of vaporization of cyclic alkylene carbonates
pvap	0.25	kPa	357.50	Vapour pressure and enthalpy of vaporization of cyclic alkylene carbonates
pvap	0.26	kPa	358.90	Vapour pressure and enthalpy of vaporization of cyclic alkylene carbonates
pvap	0.29	kPa	360.60	Vapour pressure and enthalpy of vaporization of cyclic alkylene carbonates
pvap	0.33	kPa	363.20	Vapour pressure and enthalpy of vaporization of cyclic alkylene carbonates
pvap	0.35	kPa	364.10	Vapour pressure and enthalpy of vaporization of cyclic alkylene carbonates
pvap	0.40	kPa	366.70	Vapour pressure and enthalpy of vaporization of cyclic alkylene carbonates

pvap	0.17	kPa	353.15	Low pressure methane solubility in lithium-ion batteries based solvents and electrolytes as a function of temperature. Measurement and prediction
rhol	1315.70	kg/m3	318.15	Solid-liquid equilibria and thermo-physical properties of liquid electrolyte systems for lithium ion batteries
rhol	1350.00	kg/m3	298.15	Low pressure carbon dioxide solubility in lithium-ion batteries based electrolytes as a function of temperature. Measurement and prediction
rhos	1320.00	kg/m3	293.00	Cyclic alkylene carbonates. Experiment and first principle calculations for prediction of thermochemical properties
sfust	42.96	J/mol×K	309.49	NIST Webbook
sfust	42.96	J/mol×K	309.49	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	516.70	K	98.70	NIST Webbook

Correlations

Information	Value
Property code	pvap

Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.59477e+01
Coeff. B	-5.16933e+03
Coeff. C	-6.12240e+01
Temperature range (K), min.	391.32
Temperature range (K), max.	552.31

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	9.59483e+01
Coeff. B	-1.14946e+04
Coeff. C	-1.11778e+01
Coeff. D	3.17385e-06
Temperature range (K), min.	309.55
Temperature range (K), max.	790.00

Sources

Phase Equilibria in Binary Mixtures of Water with Cyclic Alkylene Carbonates:	https://www.doi.org/10.1021/je700689w
Characterization on the exothermic behaviors of cathode materials reacted with ethylene carbonate in lithium-ion battery studied by differential scanning calorimeter (DSC):	https://www.doi.org/10.1016/j.tca.2016.09.007
Phase equilibrium and activity coefficients in ternary systems at 298.15 K: 1-propanol + ethylene carbonate + water:	https://www.doi.org/10.1016/j.jct.2016.03.027
Liquid-liquid equilibrium of 1-ethyl-3-methylimidazolium bromide ionic liquid + water + ethylene carbonate mixtures at T = (298.2, 308.2 and 318.2) K:	https://www.doi.org/10.1016/j.fluid.2019.05.015
Modified Wilson and NRTL Equation for Vapor-Liquid Equilibrium Calculations:	http://link.springer.com/article/10.1007/BF02311772
Standard partial molar volumes of some electrolytes in ethylene carbonate based mixtures:	https://www.doi.org/10.1016/j.jct.2003.09.005
Efficient determination of crystallisation and melting points at low cooling and heating rates with novel computer controlled equipment:	https://www.doi.org/10.1016/j.jct.2008.05.012
Low pressure carbon dioxide solubility in pure electrolyte solvents for lithium ion batteries as a function of temperature. Measurement and prediction:	https://www.doi.org/10.1016/j.jct.2012.01.027
Isobaric Vapor-Liquid Equilibria of Binary Mixtures Containing the Carbonate Group:	https://www.doi.org/10.1021/je049859c
Liquid-liquid equilibria for ternary mixtures of (solvent + aromatic hydrocarbon + alkane):	https://www.doi.org/10.1016/j.jct.2005.01.016
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
Liquid liquid equilibria for mixtures of (ethylene carbonate + aromatic hydrocarbon + cyclohexane):	https://www.doi.org/10.1016/j.tca.2006.03.012
Infinite Dilution Activity Coefficients in Ethylene Glycol and Ethylene Carbonate:	https://www.doi.org/10.1021/je0102107
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Vapour pressure and enthalpy of vaporization of cyclic alkylene carbonates:	https://www.doi.org/10.1016/j.fluid.2008.03.013
Separation of aromatic hydrocarbons (toluene or benzene) from aliphatic hydrocarbon (n-heptane) by extraction with ethylene carbonate:	https://www.doi.org/10.1016/j.jct.2010.05.004
Cyclic alkylene carbonates. Experiment and first principle calculations for prediction of thermochemical properties:	https://www.doi.org/10.1016/j.jct.2008.05.001
Low-pressure methane solubility in lithium-ion batteries based solvents and electrolytes as a function of temperature. Measurement and prediction:	https://www.doi.org/10.1016/j.jct.2014.07.004
KDB:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1165
Vapor Pressure and Liquid Heat Capacity of Alkylene Carbonates:	https://www.doi.org/10.1021/je034173q
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C96491&Units=SI
Measurement and Correlation of the Electrical Conductivity of the Ionic Liquid [BMIM][PF6] in Binary Organic Solvents:	https://www.doi.org/10.1021/acs.jced.7b00646
KDB Vapor Pressure Data:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1165
Low pressure carbon dioxide solubility in lithium-ion batteries based electrolytes as a function of temperature:	https://www.doi.org/10.1016/j.jct.2012.12.025
Solid-liquid equilibria and thermo-physical properties of liquid systems for lithium ion batteries:	https://www.doi.org/10.1016/j.fluid.2018.05.033
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

affp:	Proton affinity
basg:	Gas basicity
chl:	Standard liquid enthalpy of combustion
chs:	Standard solid enthalpy of combustion
cpg:	Ideal gas heat capacity
cpl:	Liquid phase heat capacity
cps:	Solid phase heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfl:	Liquid phase enthalpy of formation at standard conditions
hfs:	Solid phase enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hfust:	Enthalpy of fusion at a given temperature
hsubt:	Enthalpy of sublimation 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
pc:	Critical Pressure
pvap:	Vapor pressure
rhol:	Liquid Density
rhos:	Solid Density
sfust:	Entropy of fusion at a given temperature
ss:	Solid phase molar entropy at standard conditions
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
tt:	Triple Point Temperature
vc:	Critical Volume