ETHYL METHYL CARBONATE

Other names:	C2H5OCOOCH3
	Ethoxyacetic acid, methyl ester
Inchi:	InChI=1S/C4H8O3/c1-3-7-4(5)6-2/h3H2,1-2H3
InchiKey:	JBTWLSYIZRCDFO-UHFFFAOYSA-N
Formula:	C4H8O3
SMILES:	CCOC(=O)OC
Mol. weight [g/mol]:	104.10

Physical Properties

Property code	Value	Unit	Source
af	0.4010		Cheméo Relay (1.0)
affp	842.70	kJ/mol	NIST Webbook
basg	810.80	kJ/mol	NIST Webbook
gf	-356.12	kJ/mol	Joback Method
hf	-603.87	kJ/mol	Cheméo Relay (1.0)
hfus	10.09	kJ/mol	Joback Method
hvap	39.85	kJ/mol	Cheméo Relay (1.0)
ie	10.38	eV	Cheméo Relay (1.0)
log10ws	-0.40		Cheméo Relay (1.0)
logp	0.789		Crippen Method
mcvol	80.530	ml/mol	McGowan Method
pc	4041.50	kPa	Joback Method
tb	375.41	K	Cheméo Relay (1.0)
tc	538.44	K	Cheméo Relay (1.0)
tf	218.14	K	Efficient determination of crystallisation and melting points at low cooling and heating rates with novel computer controlled equipment
vc	0.308	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source

cpg	188.25	J/mol×K	569.26	Joback Method
cpg	149.26	J/mol×K	389.63	Joback Method
cpg	162.75	J/mol×K	449.51	Joback Method
cpg	169.33	J/mol×K	479.44	Joback Method
cpg	175.78	J/mol×K	509.38	Joback Method
cpg	182.09	J/mol×K	539.32	Joback Method
cpg	156.06	J/mol×K	419.57	Joback Method
dvisc	0.0005474	Pa×s	309.43	Joback Method
dvisc	0.0012119	Pa×s	255.96	Joback Method
dvisc	0.0007844	Pa×s	282.70	Joback Method
dvisc	0.0020724	Pa×s	229.23	Joback Method
dvisc	0.0004044	Pa×s	336.16	Joback Method
dvisc	0.0003125	Pa×s	362.90	Joback Method
dvisc	0.0002501	Pa×s	389.63	Joback Method
hfust	11.24	kJ/mol	219.40	NIST Webbook
pvap	3.66	kPa	298.15	Low pressure methane solubility in lithium-ion batteries based solvents and electrolytes as a function of temperature. Measurement and prediction
pvap	4.53	kPa	303.15	Low pressure methane solubility in lithium-ion batteries based solvents and electrolytes as a function of temperature. Measurement and prediction
pvap	1.28	kPa	282.06	Low pressure methane solubility in lithium-ion batteries based solvents and electrolytes as a function of temperature. Measurement and prediction

pvap	1.52	kPa	283.15	Low pressure methane solubility in lithium-ion batteries based solvents and electrolytes as a function of temperature. Measurement and prediction
pvap	2.01	kPa	288.15	Low pressure methane solubility in lithium-ion batteries based solvents and electrolytes as a function of temperature. Measurement and prediction
pvap	2.44	kPa	293.15	Low pressure methane solubility in lithium-ion batteries based solvents and electrolytes as a function of temperature. Measurement and prediction
pvap	18.28	kPa	333.15	Low pressure methane solubility in lithium-ion batteries based solvents and electrolytes as a function of temperature. Measurement and prediction
pvap	0.96	kPa	277.96	Low pressure methane solubility in lithium-ion batteries based solvents and electrolytes as a function of temperature. Measurement and prediction

pvap	5.80	kPa	308.15	Low pressure methane solubility in lithium-ion batteries based solvents and electrolytes as a function of temperature. Measurement and prediction
pvap	6.74	kPa	310.74	Low pressure methane solubility in lithium-ion batteries based solvents and electrolytes as a function of temperature. Measurement and prediction
pvap	7.88	kPa	314.83	Low pressure methane solubility in lithium-ion batteries based solvents and electrolytes as a function of temperature. Measurement and prediction
pvap	12.28	kPa	323.15	Low pressure methane solubility in lithium-ion batteries based solvents and electrolytes as a function of temperature. Measurement and prediction
pvap	15.26	kPa	328.15	Low pressure methane solubility in lithium-ion batteries based solvents and electrolytes as a function of temperature. Measurement and prediction

rhol	1010.00	kg/m3	298.15	Low pressure carbon dioxide solubility in lithium-ion batteries based electrolytes as a function of temperature. Measurement and prediction
rhol	1006.88	kg/m3	298.15	Solid-liquid equilibria and thermo-physical properties of liquid electrolyte systems for lithium ion batteries

Sources

Liquid-Liquid Equilibria for Ternary Systems of (Ethyl Methyl Carbonate + Methanol or Ethanol + Water) at 293.15, 303.15, and 308.15 K:	https://www.doi.org/10.1021/acs.jced.8b00543
Chemeo Relay (1.0):	
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
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C623530&Units=SI
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Experimental Isobaric Vapor-Liquid Equilibrium for Binary Systems of Ethyl Methyl Carbonate + Methanol, + Ethanol, + Dimethyl Carbonate, or + Diethyl Carbonate at 101.3 kPa:	https://www.doi.org/10.1021/je100494z
Solid-liquid equilibria and thermo-physical properties of liquid electrolyte systems for lithium ion batteries:	https://www.doi.org/10.1016/j.fluid.2018.05.033
Effect of 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
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Measurement and Correlation of Liquid Liquid Equilibrium for Quaternary Systems of Water + Methanol or Ethanol + Ethyl Methyl Carbonate + Heptane at 25 deg C:	https://www.doi.org/10.1021/acs.jced.6b01031
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
Chemeo Relay (1.0_beta):	
Low pressure carbon dioxide solubility in lithium-ion batteries based electrolytes as a function of temperature. Measurement and prediction:	https://www.doi.org/10.1016/j.jct.2012.12.025

Legend

af:	Acentric Factor
affp:	Proton affinity
basg:	Gas basicity
cpg:	Ideal gas 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
hfust:	Enthalpy of fusion at a given temperature
hvap:	Enthalpy of vaporization at standard conditions
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume