Ethylene carbonate

Other names: 1,3-Dioxacyclopentan-2-one; 2-Dioxolone; Carbonic acid, cyclic ethylene ester; Cyclic ethylene carbonate; Dioxolone-2; Ethylene carbonate; Ethylene glycol carbonate; Ethylene glycol, cyclic carbonate; Ethylenester kyseliny uhlicite; Glycol carbonate; NSC 11801; Texacar EC.

InChI: InChI=1S/C3H4O3/c4-3-5-1-2-6-3/h1-2H2

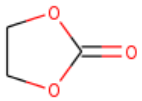
InChI Key: KMTRUDSVKNLOMY-UHFFFAOYSA-N

Formula: C3H4O3

SMILES: O=C1OCCO1

Molecular Weight: 88.06

CAS: 96-49-1



Physical Properties

Property	Value	Unit	Source
PAff	814.20	kJ/mol	NIST Webbook
BasG	784.40	kJ/mol	NIST Webbook
$\Delta_c H°_{liquid}$	-1069.30 ± 2.10	kJ/mol	NIST Webbook
$\Delta_c H°_{solid}$	-1161.40	kJ/mol	NIST Webbook
$\Delta_c H°_{solid}$	-1165.90 ± 3.70	kJ/mol	NIST Webbook
$\Delta_c H°_{solid}$	-1170.60 ± 0.40	kJ/mol	NIST Webbook
$\Delta_c H°_{solid}$	-1171.32	kJ/mol	NIST Webbook
$\Delta_f G°$	-276.19	kJ/mol	Joback Method
$\Delta_f H°_{gas}$	-503.00 ± 4.20	kJ/mol	NIST Webbook
$\Delta_f H°_{liquid}$	-682.80 ± 2.10	kJ/mol	NIST Webbook
$\Delta_f H°_{solid}$	-590.90	kJ/mol	NIST Webbook
$\Delta_f H°_{solid}$	-586.30 ± 3.80	kJ/mol	NIST Webbook
$\Delta_f H°_{solid}$	-581.60 ± 0.40	kJ/mol	NIST Webbook
$\Delta_{fus} H°$	11.86	kJ/mol	Joback Method
$\Delta_{vap} H°$	60.80 ± 0.10	kJ/mol	NIST Webbook
$\Delta_{vap} H°$	64.00 ± 0.10	kJ/mol	NIST Webbook
$\Delta_{vap} H°$	63.40 ± 0.30	kJ/mol	NIST Webbook

Property	Value	Unit	Source
$\Delta_{vap}H°$	78.50 ± 4.20	kJ/mol	NIST Webbook
$\Delta_{vap}H°$	179.80	kJ/mol	NIST Webbook
$\Delta_{vap}H°$	62.40	kJ/mol	NIST Webbook
IE	10.40	eV	NIST Webbook
IE	10.40	eV	NIST Webbook
IE	10.70	eV	NIST Webbook
IE	11.10	eV	NIST Webbook
IE	11.47	eV	NIST Webbook
$logP_{oct/wat}$	0.153		Crippen Method
P_c	6141.84	kPa	Joback Method
$S°_{solid,1\ bar}$	132.54	J/mol×K	NIST Webbook
$S°_{solid,1\ bar}$	132.54	J/mol×K	NIST Webbook
T_{boil}	516.70	K	NIST Webbook
T_c	635.21	K	Joback Method
T_{fus}	308.90 ± 0.80	K	NIST Webbook
T_{fus}	312.95 ± 0.20	K	NIST Webbook
T_{fus}	309.65 ± 0.15	K	NIST Webbook
T_{fus}	309.45 ± 0.20	K	NIST Webbook
T_{fus}	311.15 ± 1.50	K	NIST Webbook
T_{fus}	308.95 ± 0.50	K	NIST Webbook
T_{fus}	309.50 ± 0.60	K	NIST Webbook
T_{triple}	309.47 ± 0.00	K	NIST Webbook
T_{triple}	309.49 ± 0.02	K	NIST Webbook
V_c	0.195	m^3/kg-mol	Joback Method

Temperature Dependent Properties

Property	Value	Unit	Temperature (K)	Source
$C_{p,gas}$	105.45	J/mol×K	409.71	Joback Method
$C_{p,liquid}$	133.90	J/mol×K	323.15	NIST Webbook
$C_{p,solid}$	117.44	J/mol×K	298.15	NIST Webbook
$C_{p,solid}$	117.44	J/mol×K	298.15	NIST Webbook
$\Delta_{fus}H$	13.29	kJ/mol	309.49	NIST Webbook
$\Delta_{fus}H$	13.29	kJ/mol	309.49	NIST Webbook
$\Delta_{fus}H$	13.30	kJ/mol	309.5	NIST Webbook
$\Delta_{fus}H$	13.30	kJ/mol	309.5	NIST Webbook
$\Delta_{fus}H$	13.02	kJ/mol	311.2	NIST Webbook
$\Delta_{sub}H$	68.70	kJ/mol	285.0	NIST Webbook
$\Delta_{vap}H$	55.00	kJ/mol	400.5	NIST Webbook
$\Delta_{vap}H$	60.30	kJ/mol	408.5	NIST Webbook
$\Delta_{vap}H$	56.30	kJ/mol	408.5	NIST Webbook
$\Delta_{vap}H$	59.60	kJ/mol	409.0	NIST Webbook
$\Delta_{vap}H$	56.48	kJ/mol	423.0	NIST Webbook
$\Delta_{fus}S$	42.96	J/mol×K	309.49	NIST Webbook
$\Delta_{fus}S$	42.96	J/mol×K	309.49	NIST Webbook

Sources

Joback Method: https://en.wikipedia.org/wiki/Joback_method
NIST Webbook: http://webbook.nist.gov/cgi/inchi/InChI=1S/C3H4O3/c4-3-5-1-2-6-3/h1-2H2
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

PAff: Proton affinity (kJ/mol).
BasG: Gas basicity (kJ/mol).
Δ_c**H°liquid**: Standard liquid enthalpy of combustion (kJ/mol).
Δ_c**H°solid**: Standard solid enthalpy of combustion (kJ/mol).
C$_{p,gas}$: Ideal gas heat capacity (J/mol×K).
C$_{p,liquid}$: Liquid phase heat capacity (J/mol×K).

$C_{p,solid}$: Solid phase heat capacity (J/mol×K).
$\Delta_f G°$: Standard Gibbs free energy of formation (kJ/mol).
$\Delta_f H°_{gas}$: Enthalpy of formation at standard conditions (kJ/mol).
$\Delta_f H°_{liquid}$: Liquid phase enthalpy of formation at standard conditions (kJ/mol).
$\Delta_f H°_{solid}$: Solid phase enthalpy of formation at standard conditions (kJ/mol).
$\Delta_{fus} H°$: Enthalpy of fusion at standard conditions (kJ/mol).
$\Delta_{fus} H$: Enthalpy of fusion at a given temperature (kJ/mol).
$\Delta_{sub} H$: Enthalpy of sublimation at a given temperature (kJ/mol).
$\Delta_{vap} H°$: Enthalpy of vaporization at standard conditions (kJ/mol).
$\Delta_{vap} H$: Enthalpy of vaporization at a given temperature (kJ/mol).
IE: Ionization energy (eV).
***log*P$_{oct/wat}$**: Octanol/Water partition coefficient .
P_c: Critical Pressure (kPa).
$\Delta_{fus} S$: Entropy of fusion at a given temperature (J/mol×K).
$S°_{solid,1\ bar}$: Solid phase molar entropy at standard conditions (J/mol×K).
T_{boil}: Normal Boiling Point Temperature (K).
T_c: Critical Temperature (K).
T_{fus}: Normal melting (fusion) point (K).
T_{triple}: Triple Point Temperature (K).
V_c: Critical Volume (m^3/kg-mol).