Diphenyl carbonate

Other names:	Carbonic acid, diphenyl ester
	PHENYL CARBONATE
	Phenol carbonate
Inchi:	InChI=1S/C13H10O3/c14-13(15-11-7-3-1-4-8-11)16-12-9-5-2-6-10-12/h1-10H
InchiKey:	ROORDVPLFPIABK-UHFFFAOYSA-N
Formula:	C13H10O3
SMILES:	O=C(Oc1ccccc1)Oc1ccccc1
Mol. weight [g/mol]:	214.22
CAS:	102-09-0

Physical Properties

Property code	Value	Unit	Source
chs	-6143.60 ± 1.90	kJ/mol	NIST Webbook
gf	-55.52	kJ/mol	Joback Method
hf	-311.00 ± 8.80	kJ/mol	NIST Webbook
hfs	-401.40 ± 1.90	kJ/mol	NIST Webbook
hfus	21.48	kJ/mol	Joback Method
hsub	90.00 ± 8.40	kJ/mol	NIST Webbook
hsub	90.00 ± 8.40	kJ/mol	NIST Webbook
hvap	80.90 ± 0.60	kJ/mol	NIST Webbook
ie	9.01 ± 0.05	eV	NIST Webbook
log10ws	-3.69		Crippen Method
logp	3.264		Crippen Method
mcvol	159.820	ml/mol	McGowan Method
pc	3173.97	kPa	Joback Method
ss	278.40	J/mol×K	NIST Webbook
tb	579.20	K	NIST Webbook
tb	574.70	K	NIST Webbook
tc	893.05	K	Joback Method
tf	353.96	K	Solid-Liquid Equilibria in Three Binary Mixtures Containing Diphenyl Carbonate
tf	355.95	K	Solubility of Diphenyl Carbonate in Pure Alcohols from (283 to 333) K

tf	353.96	K	Solid-liquid equilibria and the physical properties of binary systems of diphenyl carbonate, dimethyl carbonate, methyl phenyl carbonate, anisole, methanol and phenol
vc	0.590	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	390.94	J/mol×K	648.91	Joback Method
cpg	405.28	J/mol×K	689.60	Joback Method
cpg	418.47	J/mol×K	730.29	Joback Method
cpg	430.54	J/mol×K	770.98	Joback Method
cpg	441.51	J/mol×K	811.67	Joback Method
cpg	451.43	J/mol×K	852.36	Joback Method
cpg	460.31	J/mol×K	893.05	Joback Method
cps	263.13	J/mol×K	298.15	NIST Webbook
dvisc	0.0001324	Pa×s	648.91	Joback Method
dvisc	0.0001676	Pa×s	604.67	Joback Method
dvisc	0.0002203	Pa×s	560.44	Joback Method
dvisc	0.0003033	Pa×s	516.20	Joback Method
dvisc	0.0004434	Pa×s	471.97	Joback Method
dvisc	0.0007012	Pa×s	427.74	Joback Method
dvisc	0.0012325	Pa×s	383.50	Joback Method
hfust	23.43	kJ/mol	355.00	NIST Webbook
psub	5.01e-05	kPa	308.17	Vapour pressures of selected organic compounds down to 1 mPa, using mass-loss Knudsen effusion method
psub	5.00e-05	kPa	308.17	Vapour pressures of selected organic compounds down to 1 mPa, using mass-loss Knudsen effusion method

psub	5.17e-05	kPa	308.17	Vapour pressures of selected organic compounds down to 1 mPa, using mass-loss Knudsen effusion method
psub	5.01e-05	kPa	308.17	Vapour pressures of selected organic compounds down to 1 mPa, using mass-loss Knudsen effusion method
psub	5.05e-05	kPa	308.17	Vapour pressures of selected organic compounds down to 1 mPa, using mass-loss Knudsen effusion method
psub	5.09e-05	kPa	308.17	Vapour pressures of selected organic compounds down to 1 mPa, using mass-loss Knudsen effusion method
psub	1.13e-04	kPa	314.32	Vapour pressures of selected organic compounds down to 1 mPa, using mass-loss Knudsen effusion method
psub	1.13e-04	kPa	314.32	Vapour pressures of selected organic compounds down to 1 mPa, using mass-loss Knudsen effusion method
psub	1.14e-04	kPa	314.32	Vapour pressures of selected organic compounds down to 1 mPa, using mass-loss Knudsen effusion method

psub	1.16e-04	kPa	314.32	Vapour pressures of selected organic compounds down to 1 mPa, using mass-loss Knudsen effusion method
psub	1.16e-04	kPa	314.32	Vapour pressures of selected organic compounds down to 1 mPa, using mass-loss Knudsen effusion method
psub	1.15e-04	kPa	314.32	Vapour pressures of selected organic compounds down to 1 mPa, using mass-loss Knudsen effusion method
psub	1.14e-04	kPa	314.32	Vapour pressures of selected organic compounds down to 1 mPa, using mass-loss Knudsen effusion method
psub	5.17e-05	kPa	308.17	Vapour pressures of selected organic compounds down to 1 mPa, using mass-loss Knudsen effusion method
psub	2.42e-04	kPa	320.25	Vapour pressures of selected organic compounds down to 1 mPa, using mass-loss Knudsen effusion method
psub	2.39e-04	kPa	320.25	Vapour pressures of selected organic compounds down to 1 mPa, using mass-loss Knudsen effusion method

psub	2.50e-04	kPa	320.25	Vapour pressures of selected organic compounds down to 1 mPa, using mass-loss Knudsen effusion method
psub	2.46e-04	kPa	320.25	Vapour pressures of selected organic compounds down to 1 mPa, using mass-loss Knudsen effusion method
psub	2.47e-04	kPa	320.25	Vapour pressures of selected organic compounds down to 1 mPa, using mass-loss Knudsen effusion method
psub	2.42e-04	kPa	320.25	Vapour pressures of selected organic compounds down to 1 mPa, using mass-loss Knudsen effusion method
psub	5.05e-04	kPa	326.23	Vapour pressures of selected organic compounds down to 1 mPa, using mass-loss Knudsen effusion method
psub	5.08e-04	kPa	326.23	Vapour pressures of selected organic compounds down to 1 mPa, using mass-loss Knudsen effusion method
psub	4.99e-04	kPa	326.23	Vapour pressures of selected organic compounds down to 1 mPa, using mass-loss Knudsen effusion method

psub	5.18e-04	kPa	326.23	Vapour pressures of selected organic compounds down to 1 mPa, using mass-loss Knudsen effusion method	
psub	5.12e-04	kPa	326.23	Vapour pressures of selected organic compounds down to 1 mPa, using mass-loss Knudsen effusion method	
psub	5.17e-04	kPa	326.23	Vapour pressures of selected organic compounds down to 1 mPa, using mass-loss Knudsen effusion method	
psub	5.07e-04	kPa	326.23	Vapour pressures of selected organic compounds down to 1 mPa, using mass-loss Knudsen effusion method	
psub	1.04e-03	kPa	332.24	Vapour pressures of selected organic compounds down to 1 mPa, using mass-loss Knudsen effusion method	
psub	1.04e-03	kPa	332.24	Vapour pressures of selected organic compounds down to 1 mPa, using mass-loss Knudsen effusion method	
psub	9.92e-04	kPa	332.24	Vapour pressures of selected organic compounds down to 1 mPa, using mass-loss Knudsen effusion method	

psub	1.06e-03	kPa	332.24	Vapour pressures of selected organic compounds down to 1 mPa, using mass-loss Knudsen effusion method
psub	1.03e-03	kPa	332.24	Vapour pressures of selected organic compounds down to 1 mPa, using mass-loss Knudsen effusion method
psub	1.07e-03	kPa	332.24	Vapour pressures of selected organic compounds down to 1 mPa, using mass-loss Knudsen effusion method
psub	2.14e-05	kPa	302.18	Vapour pressures of selected organic compounds down to 1 mPa, using mass-loss Knudsen effusion method
psub	2.22e-05	kPa	302.18	Vapour pressures of selected organic compounds down to 1 mPa, using mass-loss Knudsen effusion method
psub	2.27e-05	kPa	302.18	Vapour pressures of selected organic compounds down to 1 mPa, using mass-loss Knudsen effusion method
psub	2.27e-05	kPa	302.18	Vapour pressures of selected organic compounds down to 1 mPa, using mass-loss Knudsen effusion method

psub	2.28e-05	kPa	302.18	Vapour pressures of selected organic compounds down to 1 mPa, using mass-loss Knudsen effusion method
psub	2.20e-05	kPa	302.18	Vapour pressures of selected organic compounds down to 1 mPa, using mass-loss Knudsen effusion method
psub	2.22e-05	kPa	302.18	Vapour pressures of selected organic compounds down to 1 mPa, using mass-loss Knudsen effusion method
psub	2.40e-04	kPa	320.25	Vapour pressures of selected organic compounds down to 1 mPa, using mass-loss Knudsen effusion method
rhol	1113.14	kg/m3	358.15	Liquid Liquid Equilibria for Ternary Mixtures of Methylphenyl Carbonate, Dimethyl Carbonate, Diphenyl Carbonate, Anisole, Methanol, Phenol, and Water at Several Temperatures

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tfp	352.70	K	101.00	Solid-liquid equilibria for selected binary systems containing diphenyl carbonate

Sources

Solubility of Diphenyl Carbonate in Pure Alcohols from (283 to 333) K:	https://www.doi.org/10.1021/je800569v
Isothermal (vapour + liquid) equilibrium (VLE) for binary mixtures containing diethyl carbonate, phenyl acetate, dimethyl carbonate, or ethyl acetate:	https://www.doi.org/10.1016/j.jct.2015.07.024
Liquid-Liquid Equilibria for Ternary Mixtures of Methylphenyl Carbonate, Dimethyl Carbonate, Diphenyl Carbonate, Anisole, Methanol, Phenol, and Water at Several Temperatures:	https://www.doi.org/10.1021/je400776b
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C102090&Units=SI
Solid-liquid equilibria and the physical properties of binary systems of diphenyl carbonate, dimethyl carbonate, methyl phenyl carbonate, anisole, methanol and phenol:	https://www.doi.org/10.1016/j.fluid.2014.05.033
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Solid-Liquid Equilibria in Three Binary Mixtures Containing Diphenyl Carbonate:	https://www.doi.org/10.1021/je101199g
Vapour pressures of selected organic compounds down to 1 mPa, using mass-loss Knudsen effusion method:	https://www.doi.org/10.1016/j.jct.2013.11.038
Liquid-liquid equilibria of ternary mixtures of dimethyl carbonate, diphenyl carbonate, phenol and water at 353.15 K:	https://www.doi.org/10.1016/j.fluid.2010.11.012
Solid-liquid equilibria for selected binary systems containing diphenyl carbonate:	https://www.doi.org/10.1016/j.fluid.2018.09.023
KDB:	https://www.cheric.org/files/research/kdb/mol/mol1153.mol

Legend

chs:	Standard solid enthalpy of combustion
cpg:	Ideal gas heat capacity
cps:	Solid phase heat capacity
dvisc:	Dynamic viscosity
gf:	Standard Gibbs free energy of formation
hf:	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
hsub:	Enthalpy of sublimation at standard conditions
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
psub:	Sublimation pressure
rhol:	Liquid Density

ss:	Solid phase molar entropy at standard conditions
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
tfp:	Melting point
vc:	Critical Volume