Carbonic acid, methyl phenyl ester

Other names:	Methyl phenyl carbonate
	Phenyl methyl carbonate
Inchi:	InChI=1S/C8H8O3/c1-10-8(9)11-7-5-3-2-4-6-7/h2-6H,1H3
InchiKey:	XTBFPVLHGVYOQH-UHFFFAOYSA-N
Formula:	C8H8O3
SMILES:	COC(=O)Oc1ccccc1
Mol. weight [g/mol]:	152.15
CAS:	13509-27-8

Physical Properties

Property code	Value	Unit	Source
gf	-210.03	kJ/mol	Joback Method
hf	-348.94	kJ/mol	Joback Method
hfus	14.49	kJ/mol	Joback Method
hvap	47.24	kJ/mol	Joback Method
log10ws	-1.85		Crippen Method
logp	1.832		Crippen Method
mcvol	113.130	ml/mol	McGowan Method
pc	3782.33	kPa	Joback Method
tb	507.83	K	Joback Method
tc	725.28	K	Joback Method
tf	242.15	K	Solid-liquid equilibria and the physical properties of binary systems of diphenyl carbonate, dimethyl carbonate, methyl phenyl carbonate, anisole, methanol and phenol
vc	0.417	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	236.22	J/mol×K	507.83	Joback Method
cpg	247.47	J/mol×K	544.07	Joback Method
cpg	258.16	J/mol×K	580.31	Joback Method

cpg	268.27	J/mol×K	616.56	Joback Method
cpg	277.81	J/mol×K	652.80	Joback Method
cpg	286.77	J/mol×K	689.04	Joback Method
cpg	295.15	J/mol×K	725.28	Joback Method
dvisc	0.0010273	Pa×s	335.25	Joback Method
dvisc	0.0017691	Pa×s	300.73	Joback Method
dvisc	0.0006603	Pa×s	369.76	Joback Method
dvisc	0.0004577	Pa×s	404.28	Joback Method
dvisc	0.0003360	Pa×s	438.80	Joback Method
dvisc	0.0002581	Pa×s	473.31	Joback Method
dvisc	0.0002055	Pa×s	507.83	Joback Method
rhol	1143.63	kg/m3	298.15	Isobaric vapor-liquid equilibrium at 101.3 kPa and excess properties at 298.15 K for binary mixtures of methyl phenyl carbonate with methanol or dimethyl carbonate
rhol	1143.24	kg/m3	298.15	Liquid Liquid Equilibria for Ternary Mixtures of Methylphenyl Carbonate, Dimethyl Carbonate, Diphenyl Carbonate, Anisole, Methanol, Phenol, and Water at Several Temperatures

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Isobaric vapor-liquid equilibrium at 101.3 kPa and excess properties at 298.15 K for binary mixtures of methyl phenyl carbonate with methanol or dimethyl carbonate:	https://www.doi.org/10.1016/j.fluid.2013.09.030
Solid-liquid equilibria and thermophysical properties of binary systems of dimethyl carbonate, diphenyl carbonate, and methyl phenyl carbonate:	https://www.doi.org/10.1016/j.fluid.2014.05.033
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
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C13509278&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

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
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rhol:	Liquid Density
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume