PHENYL CHLOROFORMATE

Other names:	Carbonochloridic acid, phenyl ester
	Formic acid, chloro-, phenyl ester
	Chloroformic acid phenyl ester
	Phenoxycarbonyl chloride
	Phenyl chlorocarbonate
	Fenylester kyseliny chlormravenci
	UN 2746
	NSC 210946
Inchi:	InChI=1S/C7H5ClO2/c8-7(9)10-6-4-2-1-3-5-6/h1-5H
InchiKey:	AHWALFGBDFAJAI-UHFFFAOYSA-N
Formula:	C7H5ClO2
SMILES:	O=C(Cl)Oc1ccccc1
Mol. weight [g/mol]:	156.57

Physical Properties

Property code	Value	Unit	Source
af	0.4539		Cheméo Relay (1.0)
hf	-270.72	kJ/mol	Cheméo Relay (1.0)
hfus	14.91	kJ/mol	Joback Method
hvap	48.23	kJ/mol	Cheméo Relay (1.0)
ie	9.08	eV	Cheméo Relay (1.0)
log10ws	-2.50		Cheméo Relay (1.0)
logp	2.424		Crippen Method
mcvol	105.410	ml/mol	McGowan Method
pc	4162.33	kPa	Joback Method
tb	462.27	K	Cheméo Relay (1.0)
tc	680.08	K	Cheméo Relay (1.0)
tf	225.79	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	196.73	J/mol×K	499.96	Joback Method
cpg	245.22	J/mol×K	728.98	Joback Method

cpg	238.57	J/mol×K	690.81	Joback Method
cpg	231.37	J/mol×K	652.64	Joback Method
cpg	223.60	J/mol×K	614.47	Joback Method
cpg	215.25	J/mol×K	576.30	Joback Method
cpg	206.29	J/mol×K	538.13	Joback Method
dvisc	0.0005955	Pa×s	398.55	Joback Method
dvisc	0.0002716	Pa×s	499.96	Joback Method
dvisc	0.0003397	Pa×s	466.16	Joback Method
dvisc	0.0004400	Pa×s	432.36	Joback Method
dvisc	0.0022311	Pa×s	297.15	Joback Method
dvisc	0.0008524	Pa×s	364.75	Joback Method
dvisc	0.0013130	Pa×s	330.95	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	352.70	K	1.60	NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C1885149&Units=SI
Joback Method: https://en.wikipedia.org/wiki/Joback_method
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):
Cheméo Relay (1.0, beta):

Legend

af: Acentric Factor
cpg: Ideal gas heat capacity
dvisc: Dynamic viscosity
hf: Enthalpy of formation at standard conditions
hfus: Enthalpy of fusion 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
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point