ISOPROPYL CHLOROFORMATE

Other names:	Formic acid, chloro-, isopropyl ester
	Carbonochloride acid, 1-methylethyl ester
	Chloroformic acid isopropyl ester
	Isopropyl chlorocarbonate
	Isopropyl chloroformate
	Isopropyl chloromethanoate
	Isopropylester kyseliny chlormravenci
	UN 2407
	2-Propyl chloroformate
	1-Methylethyl chloroformate
Inchi:	InChI=1S/C4H7ClO2/c1-3(2)7-4(5)6/h3H,1-2H3
InchiKey:	IVRIRQXJSNCSPQ-UHFFFAOYSA-N
Formula:	C4H7ClO2
SMILES:	CC(C)OC(=O)Cl
Mol. weight [g/mol]:	122.55

Physical Properties

Property code	Value	Unit	Source
hf	-471.18	kJ/mol	Cheméo Relay (1.0)
hfus	9.58	kJ/mol	Joback Method
hvap	30.84	kJ/mol	Cheméo Relay (1.0)
ie	10.75	eV	Cheméo Relay (1.0)
log10ws	-1.77		Cheméo Relay (1.0)
logp	1.770		Crippen Method
mcvol	86.900	ml/mol	McGowan Method
pc	3980.54	kPa	Joback Method
tb	359.85	K	Cheméo Relay (1.0)
tc	513.51	K	Cheméo Relay (1.0)
tf	175.63	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	151.16	J/mol×K	404.20	Joback Method

cpg	158.25	J/mol×K	436.20	Joback Method
cpg	165.11	J/mol×K	468.20	Joback Method
cpg	171.74	J/mol×K	500.19	Joback Method
cpg	178.13	J/mol×K	532.19	Joback Method
cpg	184.27	J/mol×K	564.19	Joback Method
cpg	190.17	J/mol×K	596.19	Joback Method
dvisc	0.0041012	Pa×s	221.92	Joback Method
dvisc	0.0020651	Pa×s	252.30	Joback Method
dvisc	0.0012051	Pa×s	282.68	Joback Method
dvisc	0.0007807	Pa×s	313.06	Joback Method
dvisc	0.0005462	Pa×s	343.44	Joback Method
dvisc	0.0004049	Pa×s	373.82	Joback Method
dvisc	0.0003140	Pa×s	404.20	Joback Method

Sources

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):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C108236&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

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
tc:	Critical Temperature

tf: Normal melting (fusion) point