

Carbonochloridic acid, 1-methylethyl ester

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
CAS:	108-23-6

Physical Properties

Property code	Value	Unit	Source
gf	-265.49	kJ/mol	Joback Method
hf	-391.71	kJ/mol	Joback Method
hfus	9.58	kJ/mol	Joback Method
hvap	37.65	kJ/mol	Joback Method
log10ws	-1.60		Crippen Method
logp	1.770		Crippen Method
mcvol	86.900	ml/mol	McGowan Method
pc	3980.54	kPa	Joback Method
tb	404.20	K	Joback Method
tc	596.19	K	Joback Method
tf	221.92	K	Joback Method
vc	0.327	m ³ /kmol	Joback Method

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	Paxs	221.92	Joback Method
dvisc	0.0020651	Paxs	252.30	Joback Method
dvisc	0.0012051	Paxs	282.68	Joback Method
dvisc	0.0007807	Paxs	313.06	Joback Method
dvisc	0.0005462	Paxs	343.44	Joback Method
dvisc	0.0004049	Paxs	373.82	Joback Method
dvisc	0.0003140	Paxs	404.20	Joback Method

Sources

Crippen Method:

https://www.chemeo.com/doc/models/crippen_log10ws

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=C108236&Units=SI>

Crippen Method:

<http://pubs.acs.org/doi/abs/10.1021/ci9903071>

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
mccvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature

tf: Normal melting (fusion) point

vc: Critical Volume

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