Propionic acid, 2-chloro-, isopropyl ester

Other names:	2-Chloropropionic acid isopropyl ester
	Isopropyl 2-chloropropionate
	UN 2934
	Propionic acid, 2-chloro-, 1-methylethyl ester
	1-Methylethyl 2-chloropropanoate
	Propanoic acid, 2-chloro-, 1-methylethyl ester
	Isopropyl, alpha-chloro propionate
	Isopropyl 2-chloropropanoate
Inchi:	InChI=1S/C6H11ClO2/c1-4(2)9-6(8)5(3)7/h4-5H,1-3H3
InchiKey:	BOKVSRHWZPCJRN-UHFFFAOYSA-N
Formula:	C6H11ClO2
SMILES:	CC(C)OC(=O)C(C)Cl
Mol. weight [g/mol]:	150.60
CAS:	40058-87-5

Physical Properties

Property code	Value	Unit	Source
gf	-251.09	kJ/mol	Joback Method
hf	-438.27	kJ/mol	Joback Method
hfus	11.23	kJ/mol	Joback Method
hvap	41.72	kJ/mol	Joback Method
log10ws	-1.57		Crippen Method
logp	1.565		Crippen Method
mcvol	115.080	ml/mol	McGowan Method
pc	3195.54	kPa	Joback Method
rinpol	866.00		NIST Webbook
rinpol	886.00		NIST Webbook
rinpol	885.00		NIST Webbook
rinpol	880.00		NIST Webbook
rinpol	876.00		NIST Webbook
rinpol	873.00		NIST Webbook
rinpol	873.00		NIST Webbook
rinpol	876.00		NIST Webbook
rinpol	876.00		NIST Webbook
ripol	1226.00		NIST Webbook
ripol	1216.00		NIST Webbook
ripol	1233.00		NIST Webbook

ripol	1264.00		NIST Webbook
ripol	1229.00		NIST Webbook
tb	449.52	K	Joback Method
tc	642.38	K	Joback Method
tf	229.46	K	Joback Method
vc	0.432	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	225.19	J/mol×K	449.52	Joback Method
cpg	235.42	J/mol×K	481.66	Joback Method
cpg	245.24	J/mol×K	513.81	Joback Method
cpg	254.67	J/mol×K	545.95	Joback Method
cpg	263.70	J/mol×K	578.09	Joback Method
cpg	272.33	J/mol×K	610.24	Joback Method
cpg	280.57	J/mol×K	642.38	Joback Method
dvisc	0.0065779	Pa×s	229.46	Joback Method
dvisc	0.0026871	Pa×s	266.14	Joback Method
dvisc	0.0013635	Pa×s	302.81	Joback Method
dvisc	0.0008011	Pa×s	339.49	Joback Method
dvisc	0.0005221	Pa×s	376.17	Joback Method
dvisc	0.0003672	Pa×s	412.84	Joback Method
dvisc	0.0002735	Pa×s	449.52	Joback Method

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=C40058875&Units=SI

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
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume