ClCH2C(O)OCH(CH3)2

Other names:	Acetic acid, chloro-, 1-methylethyl ester
	Acetic acid, chloro-, isopropyl ester
	Chloroacetic acid isopropyl ester
	Chloroacetic acid, 1-methyl ester
	Isopropyl chloroacetate
	Monochloroacetic acid isopropyl ester
	UN 2947
Inchi:	InChI=1S/C5H9ClO2/c1-4(2)8-5(7)3-6/h4H,3H2,1-2H3
InchiKey:	VODRWDBLLGYRJT-UHFFFAOYSA-N
Formula:	C5H9ClO2
SMILES:	CC(C)OC(=O)CCl
Mol. weight [g/mol]:	136.58
CAS:	105-48-6

Physical Properties

Property code	Value	Unit	Source
chl	-2733.00	kJ/mol	NIST Webbook
chs	-2735.00 ± 8.00	kJ/mol	NIST Webbook
gf	-257.07	kJ/mol	Joback Method
hf	-412.35	kJ/mol	Joback Method
hfus	12.17	kJ/mol	Joback Method
hvap	38.00	kJ/mol	NIST Webbook
log10ws	-1.04		Crippen Method
logp	1.177		Crippen Method
mcvol	100.990	ml/mol	McGowan Method
pc	3538.87	kPa	Joback Method
rinpol	850.00		NIST Webbook
rinpol	891.00		NIST Webbook
rinpol	861.00		NIST Webbook
rinpol	845.00		NIST Webbook
rinpol	880.00		NIST Webbook
rinpol	850.00		NIST Webbook
rinpol	850.70		NIST Webbook
rinpol	845.00		NIST Webbook
rinpol	845.00		NIST Webbook
rinpol	891.00		NIST Webbook
ripol	1280.00		NIST Webbook

ripol	1280.00		NIST Webbook
tb	423.70	K	NIST Webbook
tc	617.43	K	Joback Method
tf	233.19	K	Joback Method
vc	0.383	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	186.92	J/mol×K	427.08	Joback Method
cpg	195.50	J/mol×K	458.81	Joback Method
cpg	203.77	J/mol×K	490.53	Joback Method
cpg	211.73	J/mol×K	522.26	Joback Method
cpg	219.39	J/mol×K	553.98	Joback Method
cpg	226.73	J/mol×K	585.71	Joback Method
cpg	233.77	J/mol×K	617.43	Joback Method
dvisc	0.0042591	Pa×s	233.19	Joback Method
dvisc	0.0020958	Pa×s	265.50	Joback Method
dvisc	0.0012028	Pa×s	297.82	Joback Method
dvisc	0.0007696	Pa×s	330.13	Joback Method
dvisc	0.0005332	Pa×s	362.45	Joback Method
dvisc	0.0003923	Pa×s	394.76	Joback Method
dvisc	0.0003024	Pa×s	427.08	Joback Method
hvapt	44.30	kJ/mol	366.50	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.49438e+01
Coeff. B	-4.87503e+03
Coeff. C	1.78690e+01
Temperature range (K), min.	271.15
Temperature range (K), max.	488.24

Sources

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=C105486&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

chl:	Standard liquid enthalpy of combustion
chs:	Standard solid enthalpy of combustion
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
hvapt:	Enthalpy of vaporization at a given temperature
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
pvap:	Vapor 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