Carbonochloridic acid, ethyl ester

Other names:	CATHYL CHLORIDE
	Chlorocarbonate d'ethyle
	Chlorocarbonic acid, ethyl ester
	Chloroformic acid, ethyl ester
	Clhorameisensaeureaethylester
	ECF
	ETHOXYCARBONYL CHLORIDE
	Ethyl carbonochloridate
	Ethyl chlorocarbonate
	Ethyl chloroformate
	Ethylchloorformiaat
	Ethyle, chloroformiat d'
	Ethylester kyseliny chlormravenci
	Etil clorocarbonato
	Etil cloroformiato
	Formic acid, chloro-, ethyl ester
	TL 423
	UN 1182
Inchi:	InChI=1S/C3H5ClO2/c1-2-6-3(4)5/h2H2,1H3
InchiKey:	RIFGWPKJUGCATF-UHFFFAOYSA-N
Formula:	C3H5ClO2
SMILES:	CCOC(=O)Cl
Mol. weight [g/mol]:	108.52
CAS:	541-41-3

Physical Properties

Property code	Value	Unit	Source
affp	764.80	kJ/mol	NIST Webbook
basg	733.80	kJ/mol	NIST Webbook
chl	-1370.00 ± 4.00	kJ/mol	NIST Webbook
gf	-271.47	kJ/mol	Joback Method
hf	-459.40 ± 1.70	kJ/mol	NIST Webbook
hfl	-497.30 ± 1.70	kJ/mol	NIST Webbook
hfus	10.51	kJ/mol	Joback Method
hvap	37.80 ± 0.20	kJ/mol	NIST Webbook
hvap	37.86 ± 0.29	kJ/mol	NIST Webbook
log10ws	-1.07		Crippen Method

logp	1.382		Crippen Method
mcvol	72.810	ml/mol	McGowan Method
nfpaf	%!d(float64=3)		KDB
nfpas	%!d(float64=1)		KDB
pc	4462.28	kPa	Joback Method
rinpol	640.00		NIST Webbook
rinpol	640.00		NIST Webbook
tb	366.20	K	NIST Webbook
tc	508.15 ± 10.00	K	NIST Webbook
tf	225.65	K	Joback Method
vc	0.277	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	117.88	J/mol×K	381.76	Joback Method
cpg	123.10	J/mol×K	413.21	Joback Method
cpg	128.19	J/mol×K	444.67	Joback Method
cpg	133.14	J/mol×K	476.12	Joback Method
cpg	137.95	J/mol×K	507.57	Joback Method
cpg	142.60	J/mol×K	539.02	Joback Method
cpg	147.10	J/mol×K	570.48	Joback Method
dvisc	0.0025693	Pa×s	225.65	Joback Method
dvisc	0.0015292	Pa×s	251.67	Joback Method
dvisc	0.0010031	Pa×s	277.69	Joback Method
dvisc	0.0007073	Pa×s	303.70	Joback Method
dvisc	0.0005270	Pa×s	329.72	Joback Method
dvisc	0.0004099	Pa×s	355.74	Joback Method
dvisc	0.0003300	Pa×s	381.76	Joback Method
hvapt	38.70 ± 0.20	kJ/mol	283.50	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.65113e+01
Coeff. B	-3.62502e+03

Coeff. C	-6.13970e+01
Temperature range (K), min.	284.84
Temperature range (K), max.	508.15

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
KDB:	https://www.cheric.org/files/research/kdb/mol/mol1784.mol
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C541413&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

affp:	Proton affinity
basg:	Gas basicity
chl:	Standard liquid 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
hfl:	Liquid phase 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
nfpaf:	NFPA Fire Rating
nfpas:	NFPA Safety Rating
pc:	Critical Pressure
pvap:	Vapor pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point

vc: Critical Volume