Carbonochloridic acid, methyl ester

Other names:	Chlorameisensaeure methylester
	Chlorocarbonate de methyle
	Chlorocarbonic acid, methyl ester
	Chloroformiate de methyle
	Chloroformic acid methyl ester
	Formic acid, chloro-, methyl ester
	MCF
	Methoxycarbonyl chloride
	Methyl chlorocarbonate
	Methylchloorformiaat
	Methylester kyseliny chlormravenci
	Methylester kyseliny chloruhlicite
	Metilcloroformiato
	Rcra waste number U156
	TL 438
	UN 1238
Inchi:	InChI=1S/C2H3ClO2/c1-5-2(3)4/h1H3
InchiKey:	XMJHPCRAQCTCFT-UHFFFAOYSA-N
Formula:	C2H3ClO2
SMILES:	COC(=O)Cl
Mol. weight [g/mol]:	94.50

Physical Properties

Property code	Value	Unit	Source
af	0.3107		Cheméo Relay (1.0)
gf	-279.89	kJ/mol	Joback Method
hf	-408.67	kJ/mol	Cheméo Relay (1.0)
hfus	7.92	kJ/mol	Joback Method
hvap	25.65	kJ/mol	Cheméo Relay (1.0)
ie	11.09	eV	Cheméo Relay (1.0)
log10ws	-0.84		Cheméo Relay (1.0)
logp	0.992		Crippen Method
mcvol	58.720	ml/mol	McGowan Method
pc	5094.76	kPa	Joback Method
rinpol	582.00		NIST Webbook
rinpol	582.00		NIST Webbook
rinpol	569.00		NIST Webbook

tb	343.70	K	NIST Webbook
tc	491.78	K	Cheméo Relay (1.0)
tf	172.06	K	Cheméo Relay (1.0)
vc	0.214	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	87.27	J/mol×K	358.88	Joback Method
cpg	90.74	J/mol×K	390.48	Joback Method
cpg	94.16	J/mol×K	422.08	Joback Method
cpg	97.52	J/mol×K	453.68	Joback Method
cpg	100.81	J/mol×K	485.28	Joback Method
cpg	104.04	J/mol×K	516.88	Joback Method
cpg	107.18	J/mol×K	548.48	Joback Method
dvisc	0.0022907	Pa×s	214.38	Joback Method
dvisc	0.0014045	Pa×s	238.46	Joback Method
dvisc	0.0009420	Pa×s	262.55	Joback Method
dvisc	0.0006757	Pa×s	286.63	Joback Method
dvisc	0.0005103	Pa×s	310.71	Joback Method
dvisc	0.0004012	Pa×s	334.80	Joback Method
dvisc	0.0003258	Pa×s	358.88	Joback Method

Sources

Joback Method: https://en.wikipedia.org/wiki/Joback_method
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):
KDB: https://www.cheric.org/files/research/kdb/mol/mol1777.mol
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C79221&Units=SI

Legend

af:	Acentric Factor
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
ie:	Ionization energy
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume