Butanoic acid, 2-chloro-3-oxo-, ethyl ester

Other names:	Acetoacetic acid, 2-chloro-, ethyl ester
	Ethyl «alpha»-chloroacetoacetate
	Ethyl 2-chloracetoacetate
	Ethyl 2-chloro-3-oxobutanoate
	Ethyl 2-chloroacetoacetate
	2-Chloro-3-oxobutanoic acid, ethyl ester
	2-Chloro-3-oxobutyric acid ethyl ester
	2-Chloroacetoacetic acid ethyl ester
	A 21960
	NSC 78426
Inchi:	InChI=1S/C6H9ClO3/c1-3-10-6(9)5(7)4(2)8/h5H,3H2,1-2H3
InchiKey:	RDULEYWUGKOCMR-UHFFFAOYSA-N
Formula:	C6H9ClO3
SMILES:	CCOC(=O)C(Cl)C(C)=O
Mol. weight [g/mol]:	164.59
CAS:	609-15-4

Physical Properties

Property code	Value	Unit	Source
gf	-377.57	kJ/mol	Joback Method
hf	-545.57	kJ/mol	Joback Method
hfus	16.36	kJ/mol	Joback Method
hvap	48.85	kJ/mol	Joback Method
log10ws	-0.74		Crippen Method
logp	0.746		Crippen Method
mcvol	116.650	ml/mol	McGowan Method
pc	3403.91	kPa	Joback Method
tb	503.83	K	Joback Method
tc	702.55	K	Joback Method
tf	294.39	K	Joback Method
vc	0.445	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	238.65	J/mol×K	503.83	Joback Method
cpg	280.78	J/mol×K	669.43	Joback Method
cpg	273.17	J/mol×K	636.31	Joback Method
cpg	265.15	J/mol×K	603.19	Joback Method
cpg	256.72	J/mol×K	570.07	Joback Method
cpg	247.89	J/mol×K	536.95	Joback Method
cpg	287.98	J/mol×K	702.55	Joback Method
dvisc	0.0003108	Pa×s	503.83	Joback Method
dvisc	0.0003995	Pa×s	468.92	Joback Method
dvisc	0.0005346	Pa×s	434.02	Joback Method
dvisc	0.0007529	Pa×s	399.11	Joback Method
dvisc	0.0011322	Pa×s	364.20	Joback Method
dvisc	0.0018565	Pa×s	329.30	Joback Method
dvisc	0.0034229	Pa×s	294.39	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	380.20	K	1.90	NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C609154&Units=SI
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

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
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume