Butanoic acid, 4-chloro-3-oxo-, methyl ester

Other names:	Acetoacetic acid, 4-chloro-, methyl ester
	«gamma»-Chloroacetoacetic acid, methyl ester
	Methyl «gamma»-chloroacetoacetate
	Methyl «omega»-chloroacetoacetate
	Methyl 4-chloroacetoacetate
	methyl 4-chloro-3-oxobutyrate
Inchi:	InChI=1S/C5H7ClO3/c1-9-5(8)2-4(7)3-6/h2-3H2,1H3
InchiKey:	HFLMYYLFSNEOOT-UHFFFAOYSA-N
Formula:	C5H7ClO3
SMILES:	COC(=O)CC(=O)CCl
Mol. weight [g/mol]:	150.56
CAS:	32807-28-6

Physical Properties

Property code	Value	Unit	Source
gf	-383.55	kJ/mol	Joback Method
hf	-519.65	kJ/mol	Joback Method
hfus	17.29	kJ/mol	Joback Method
hvap	47.01	kJ/mol	Joback Method
log10ws	-0.21		Crippen Method
logp	0.357		Crippen Method
mcvol	102.560	ml/mol	McGowan Method
pc	3782.33	kPa	Joback Method
tb	481.39	K	Joback Method
tc	678.32	K	Joback Method
tf	298.12	K	Joback Method
vc	0.395	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	198.25	J/mol×K	481.39	Joback Method
cpg	205.97	J/mol×K	514.21	Joback Method
cpg	213.38	J/mol×K	547.03	Joback Method

cpg	220.47	J/mol×K	579.85	Joback Method
cpg	227.25	J/mol×K	612.68	Joback Method
cpg	233.70	J/mol×K	645.50	Joback Method
cpg	239.83	J/mol×K	678.32	Joback Method
dvisc	0.0026104	Pa×s	298.12	Joback Method
dvisc	0.0016016	Pa×s	328.67	Joback Method
dvisc	0.0010678	Pa×s	359.21	Joback Method
dvisc	0.0007586	Pa×s	389.75	Joback Method
dvisc	0.0005664	Pa×s	420.30	Joback Method
dvisc	0.0004399	Pa×s	450.85	Joback Method
dvisc	0.0003529	Pa×s	481.39	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	358.20	K	0.50	NIST Webbook

Sources

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=C32807286&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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