

Butanoic acid, 4-chloro-4-oxo-, ethyl ester

Other names:	Propionic acid, 3-(chloroformyl)-, ethyl ester «beta»-Carbethoxypropionyl chloride «beta»-Ethoxycarbonylpropionyl chloride Ethyl succinoyl chloride Ethyl succinyl chloride Ethyl 3-(chloroformyl)propionate 3-Carboethoxypropionyl chloride Ethyl 4-chloro-4-oxobutanoate
Inchi:	InChI=1S/C6H9ClO3/c1-2-10-6(9)4-3-5(7)8/h2-4H2,1H3
InchiKey:	IXZFDJXHLQQSGQ-UHFFFAOYSA-N
Formula:	C6H9ClO3
SMILES:	CCOC(=O)CCC(=O)Cl
Mol. weight [g/mol]:	164.59
CAS:	14794-31-1

Physical Properties

Property code	Value	Unit	Source
gf	-375.13	kJ/mol	Joback Method
hf	-540.29	kJ/mol	Joback Method
hfus	19.88	kJ/mol	Joback Method
hvap	49.24	kJ/mol	Joback Method
log10ws	-1.12		Crippen Method
logp	1.095		Crippen Method
mcvol	116.650	ml/mol	McGowan Method
pc	3372.36	kPa	Joback Method
tb	504.27	K	Joback Method
tc	698.73	K	Joback Method
tf	309.39	K	Joback Method
vc	0.451	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	238.35	J/molxK	504.27	Joback Method

cpg	247.32	J/molxK	536.68	Joback Method
cpg	255.91	J/molxK	569.09	Joback Method
cpg	264.12	J/molxK	601.50	Joback Method
cpg	271.94	J/molxK	633.91	Joback Method
cpg	279.39	J/molxK	666.32	Joback Method
cpg	286.45	J/molxK	698.73	Joback Method
dvisc	0.0026181	Paxs	309.39	Joback Method
dvisc	0.0015720	Paxs	341.87	Joback Method
dvisc	0.0010312	Paxs	374.35	Joback Method
dvisc	0.0007236	Paxs	406.83	Joback Method
dvisc	0.0005350	Paxs	439.31	Joback Method
dvisc	0.0004124	Paxs	471.79	Joback Method
dvisc	0.0003287	Paxs	504.27	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	362.20	K	1.50	NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=C14794311&Units=SI

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

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