3-Chloropropanoic acid butyl ester

Other names:	Propanoic acid, 3-chloro-, butyl ester
	3-Chloropropionic acid, butyl ester
	Butyl 3-chloropropanoate
	n-Butyl 3-chloropropionate
	butyl 3-chloropropionate
Inchi:	InChI=1S/C7H13ClO2/c1-2-3-6-10-7(9)4-5-8/h2-6H2,1H3
InchiKey:	KRZKQEQBZXWCDJ-UHFFFAOYSA-N
Formula:	C7H13ClO2
SMILES:	CCCCOC(=O)CCCl
Mol. weight [g/mol]:	164.63
CAS:	27387-79-7

Physical Properties

Property code	Value	Unit	Source
chl	-4078.10 ± 8.40	kJ/mol	NIST Webbook
chl	-4070.00	kJ/mol	NIST Webbook
gf	-237.79	kJ/mol	Joback Method
hf	-502.50 ± 9.60	kJ/mol	NIST Webbook
hfl	-558.10 ± 8.40	kJ/mol	NIST Webbook
hfus	20.87	kJ/mol	Joback Method
hvap	55.60 ± 4.20	kJ/mol	NIST Webbook
log10ws	-1.77		Crippen Method
logp	1.959		Crippen Method
mcvol	129.170	ml/mol	McGowan Method
pc	2826.33	kPa	Joback Method
rinpol	1098.00		NIST Webbook
rinpol	1093.00		NIST Webbook
rinpol	1092.00		NIST Webbook
rinpol	1086.00		NIST Webbook
rinpol	1085.00		NIST Webbook
rinpol	1094.00		NIST Webbook
rinpol	1083.00		NIST Webbook
rinpol	1097.00		NIST Webbook
rinpol	1091.00		NIST Webbook
ripol	1582.00		NIST Webbook
ripol	1586.00		NIST Webbook
ripol	1605.00		NIST Webbook

ripol	1558.00		NIST Webbook
ripol	1542.00		NIST Webbook
ripol	1580.00		NIST Webbook
ripol	1558.00		NIST Webbook
ripol	1544.00		NIST Webbook
tb	473.28	K	Joback Method
tc	655.90	K	Joback Method
tf	270.73	K	Joback Method
vc	0.500	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	265.22	J/mol×K	473.28	Joback Method
cpg	315.13	J/mol×K	625.46	Joback Method
cpg	305.96	J/mol×K	595.03	Joback Method
cpg	296.38	J/mol×K	564.59	Joback Method
cpg	286.40	J/mol×K	534.15	Joback Method
cpg	276.01	J/mol×K	503.72	Joback Method
cpg	323.90	J/mol×K	655.90	Joback Method
dvisc	0.0002820	Pa×s	473.28	Joback Method
dvisc	0.0003603	Pa×s	439.52	Joback Method
dvisc	0.0004794	Pa×s	405.76	Joback Method
dvisc	0.0006719	Pa×s	372.00	Joback Method
dvisc	0.0010072	Pa×s	338.25	Joback Method
dvisc	0.0016518	Pa×s	304.49	Joback Method
dvisc	0.0030645	Pa×s	270.73	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C27387797&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

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Legend

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
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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume