3-Chloropropanoic acid 3-methylbutyl ester

Other names: Propanoic acid, 3-chloro-, 3-methylbutyl ester
3-Chloropropionic acid, 3-methylbutyl ester
3-Methylbutyl 3-chloropropionate
Inchi: InChI=1S/C8H15ClO2/c1-7(2)4-6-11-8(10)3-5-9/h7H,3-6H2,1-2H3
InchiKey: ZFNWFRKLGAIOME-UHFFFAOYSA-N
Formula: C8H15ClO2
SMILES: CC(C)CCOC(=O)CCCl
Mol. weight [g/mol]: 178.66
CAS: 62108-70-7

Physical Properties

Property code	Value	Unit	Source
chl	-4722.10 ± 8.40	kJ/mol	NIST Webbook
chl	-4713.30	kJ/mol	NIST Webbook
gf	-231.81	kJ/mol	Joback Method
hf	-539.30 ± 9.60	kJ/mol	NIST Webbook
hfl	-593.30 ± 8.40	kJ/mol	NIST Webbook
hfus	19.94	kJ/mol	Joback Method
hvap	54.00 ± 4.20	kJ/mol	NIST Webbook
log10ws	-1.95		Crippen Method
logp	2.205		Crippen Method
mcvol	143.260	ml/mol	McGowan Method
pc	2579.34	kPa	Joback Method
rinpol	1148.00		NIST Webbook
rinpol	1160.00		NIST Webbook
rinpol	1160.00		NIST Webbook
rinpol	1156.00		NIST Webbook
rinpol	1155.00		NIST Webbook
rinpol	1160.00		NIST Webbook
rinpol	1166.00		NIST Webbook
rinpol	1144.00		NIST Webbook
rinpol	1148.00		NIST Webbook
ripol	1595.00		NIST Webbook
ripol	1605.00		NIST Webbook
ripol	1594.00		NIST Webbook
ripol	1594.00		NIST Webbook
ripol	1592.00		NIST Webbook

tb	495.72	K	Joback Method
tc	680.38	K	Joback Method
tf	267.00	K	Joback Method
vc	0.550	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	307.89	J/mol×K	495.72	Joback Method
cpg	363.91	J/mol×K	649.60	Joback Method
cpg	353.67	J/mol×K	618.82	Joback Method
cpg	342.95	J/mol×K	588.05	Joback Method
cpg	331.75	J/mol×K	557.27	Joback Method
cpg	320.07	J/mol×K	526.50	Joback Method
cpg	373.67	J/mol×K	680.38	Joback Method
dvisc	0.0002478	Pa×s	495.72	Joback Method
dvisc	0.0003265	Pa×s	457.60	Joback Method
dvisc	0.0004523	Pa×s	419.48	Joback Method
dvisc	0.0006687	Pa×s	381.36	Joback Method
dvisc	0.0010785	Pa×s	343.24	Joback Method
dvisc	0.0019599	Pa×s	305.12	Joback Method
dvisc	0.0042242	Pa×s	267.00	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C62108707&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