Propyl 3-chlorobutanoate

Other names: Butanoic acid, 3-chloro, propyl ester
n-Propyl 3-chlorobutyrate
Inchi: InChI=1S/C7H13ClO2/c1-3-4-10-7(9)5-6(2)8/h6H,3-5H2,1-2H3
InchiKey: OPZLOOXQPPMSKG-UHFFFAOYSA-N
Formula: C7H13ClO2
SMILES: CCCOC(=O)CC(C)Cl
Mol. weight [g/mol]: 164.63
CAS: 62108-72-9

Physical Properties

Property code	Value	Unit	Source
chl	-4045.90 ± 8.40	kJ/mol	NIST Webbook
chl	-4039.00	kJ/mol	NIST Webbook
gf	-240.23	kJ/mol	Joback Method
hf	-538.10 ± 9.60	kJ/mol	NIST Webbook
hfl	-590.40 ± 8.40	kJ/mol	NIST Webbook
hfus	17.35	kJ/mol	Joback Method
hvap	52.30 ± 4.20	kJ/mol	NIST Webbook
log10ws	-1.88		Crippen Method
logp	1.957		Crippen Method
mcvol	129.170	ml/mol	McGowan Method
pc	2850.52	kPa	Joback Method
rinpol	1043.00		NIST Webbook
rinpol	1030.00		NIST Webbook
rinpol	1045.00		NIST Webbook
rinpol	1050.00		NIST Webbook
tb	472.84	K	Joback Method
tc	659.46	K	Joback Method
tf	255.73	K	Joback Method
vc	0.494	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source

cpg	265.41	J/mol×K	472.84	Joback Method
cpg	276.52	J/mol×K	503.94	Joback Method
cpg	287.19	J/mol×K	535.05	Joback Method
cpg	297.44	J/mol×K	566.15	Joback Method
cpg	307.25	J/mol×K	597.25	Joback Method
cpg	316.63	J/mol×K	628.35	Joback Method
cpg	325.59	J/mol×K	659.46	Joback Method
dvisc	0.0043091	Pa×s	255.73	Joback Method
dvisc	0.0020358	Pa×s	291.92	Joback Method
dvisc	0.0011348	Pa×s	328.10	Joback Method
dvisc	0.0007104	Pa×s	364.28	Joback Method
dvisc	0.0004840	Pa×s	400.47	Joback Method
dvisc	0.0003514	Pa×s	436.65	Joback Method
dvisc	0.0002680	Pa×s	472.84	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C62108729&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

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

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