3-Chloropropanoic acid, 2-butyl ester

Other names: Propanoic acid, 3-chloro, 1-methylpropyl ester
Inchi: InChI=1S/C7H13ClO2/c1-3-6(2)10-7(9)4-5-8/h6H,3-5H2,1-2H3
InchiKey: XLIOZHNKYDPTAJ-UHFFFAOYSA-N
Formula: C7H13ClO2
SMILES: CCC(C)OC(=O)CCCl
Mol. weight [g/mol]: 164.63
CAS: 88736-65-6

Physical Properties

Property code	Value	Unit	Source
gf	-240.23	kJ/mol	Joback Method
hf	-453.63	kJ/mol	Joback Method
hfus	17.35	kJ/mol	Joback Method
hvap	44.33	kJ/mol	Joback Method
log10ws	-1.88		Crippen Method
logp	1.957		Crippen Method
mcvol	129.170	ml/mol	McGowan Method
pc	2850.52	kPa	Joback Method
rinpol	1033.00		NIST Webbook
rinpol	1042.00		NIST Webbook
rinpol	1033.00		NIST Webbook
rinpol	1043.00		NIST Webbook
rinpol	1038.00		NIST Webbook
rinpol	1050.00		NIST Webbook
ripol	1460.00		NIST Webbook
ripol	1471.00		NIST Webbook
ripol	1461.00		NIST Webbook
ripol	1459.00		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

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=C88736656&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
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