1-Propanol, 3-chloro, butanoate

Inchi: InChI=1S/C7H13ClO2/c1-2-4-7(9)10-6-3-5-8/h2-6H2,1H3
InchiKey: QUBZBHHDHWVMSW-UHFFFAOYSA-N
Formula: C7H13ClO2
SMILES: CCCC(=O)OCCCCl
Mol. weight [g/mol]: 164.63

Physical Properties

Property code	Value	Unit	Source
gf	-237.79	kJ/mol	Joback Method
hf	-448.35	kJ/mol	Joback Method
hfus	20.87	kJ/mol	Joback Method
hvap	44.72	kJ/mol	Joback Method
log10ws	-1.77		Crippen Method
logp	1.959		Crippen Method
mcvol	129.170	ml/mol	McGowan Method
pc	2826.33	kPa	Joback Method
rinpol	1104.00		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	276.01	J/mol×K	503.72	Joback Method
cpg	286.40	J/mol×K	534.15	Joback Method
cpg	296.38	J/mol×K	564.59	Joback Method
cpg	305.96	J/mol×K	595.03	Joback Method
cpg	315.13	J/mol×K	625.46	Joback Method
cpg	323.90	J/mol×K	655.90	Joback Method
dvisc	0.0030645	Pa×s	270.73	Joback Method
dvisc	0.0016518	Pa×s	304.49	Joback Method

dvisc	0.0010072	Pa×s	338.25	Joback Method
dvisc	0.0006719	Pa×s	372.00	Joback Method
dvisc	0.0004794	Pa×s	405.76	Joback Method
dvisc	0.0003603	Pa×s	439.52	Joback Method
dvisc	0.0002820	Pa×s	473.28	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=R34262&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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