1-Propanol, 3-chloro, propanoate

Other names: 1-Propanol, 3-chloro, propionate
Inchi: InChI=1S/C6H11ClO2/c1-2-6(8)9-5-3-4-7/h2-5H2,1H3
InchiKey: HSOLEQBYEIZXJH-UHFFFAOYSA-N
Formula: C6H11ClO2
SMILES: CCC(=O)OCCCCl
Mol. weight [g/mol]: 150.60

Physical Properties

Property code	Value	Unit	Source
gf	-246.21	kJ/mol	Joback Method
hf	-427.71	kJ/mol	Joback Method
hfus	18.28	kJ/mol	Joback Method
hvap	42.49	kJ/mol	Joback Method
log10ws	-1.35		Crippen Method
logp	1.568		Crippen Method
mcvol	115.080	ml/mol	McGowan Method
pc	3138.51	kPa	Joback Method
rinpol	1016.00		NIST Webbook
rinpol	1016.00		NIST Webbook
tb	450.40	K	Joback Method
tc	634.77	K	Joback Method
tf	259.46	K	Joback Method
vc	0.445	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	224.90	J/mol×K	450.40	Joback Method
cpg	234.51	J/mol×K	481.13	Joback Method
cpg	243.77	J/mol×K	511.86	Joback Method
cpg	252.68	J/mol×K	542.58	Joback Method
cpg	261.25	J/mol×K	573.31	Joback Method
cpg	269.47	J/mol×K	604.04	Joback Method
cpg	277.34	J/mol×K	634.77	Joback Method

dvisc	0.0030315	Pa×s	259.46	Joback Method
dvisc	0.0016707	Pa×s	291.28	Joback Method
dvisc	0.0010354	Pa×s	323.11	Joback Method
dvisc	0.0006992	Pa×s	354.93	Joback Method
dvisc	0.0005036	Pa×s	386.75	Joback Method
dvisc	0.0003813	Pa×s	418.58	Joback Method
dvisc	0.0003003	Pa×s	450.40	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R34333&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

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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