

1-Propanol, 3-chloro, hexanoate

Other names:	Hexanoic acid, 3-chloropropyl ester
Inchi:	InChI=1S/C9H17ClO2/c1-2-3-4-6-9(11)12-8-5-7-10/h2-8H2,1H3
InchiKey:	QBAPUBKDRNQWDF-UHFFFAOYSA-N
Formula:	C9H17ClO2
SMILES:	CCCCCC(=O)OCCCCI
Mol. weight [g/mol]:	192.68

Physical Properties

Property code	Value	Unit	Source
gf	-220.95	kJ/mol	Joback Method
hf	-489.63	kJ/mol	Joback Method
hfus	26.05	kJ/mol	Joback Method
hvap	49.17	kJ/mol	Joback Method
log10ws	-2.61		Crippen Method
logp	2.739		Crippen Method
mvol	157.350	ml/mol	McGowan Method
pc	2327.03	kPa	Joback Method
rinpol	1302.00		NIST Webbook
rinpol	1314.00		NIST Webbook
tb	519.04	K	Joback Method
tc	698.13	K	Joback Method
tf	293.27	K	Joback Method
vc	0.613	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	352.11	J/molxK	519.04	Joback Method
cpg	364.91	J/molxK	548.89	Joback Method
cpg	377.20	J/molxK	578.74	Joback Method
cpg	388.97	J/molxK	608.58	Joback Method
cpg	400.25	J/molxK	638.43	Joback Method
cpg	411.03	J/molxK	668.28	Joback Method
cpg	421.32	J/molxK	698.13	Joback Method

dvisc	0.0029830	Paxs	293.27	Joback Method
dvisc	0.0015445	Paxs	330.90	Joback Method
dvisc	0.0009148	Paxs	368.53	Joback Method
dvisc	0.0005970	Paxs	406.15	Joback Method
dvisc	0.0004189	Paxs	443.78	Joback Method
dvisc	0.0003106	Paxs	481.41	Joback Method
dvisc	0.0002406	Paxs	519.04	Joback Method

Sources

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=R34294&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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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