

3-Chloropropyl isohexanoate

Other names:	1-Propanol, 3-chloro, 4-methylpentanoate
Inchi:	InChI=1S/C9H17ClO2/c1-8(2)4-5-9(11)12-7-3-6-10/h8H,3-7H2,1-2H3
InchiKey:	ZUBSCVXXACFAIJ-UHFFFAOYSA-N
Formula:	C9H17ClO2
SMILES:	CC(C)CCC(=O)OCCCCl
Mol. weight [g/mol]:	192.68

Physical Properties

Property code	Value	Unit	Source
gf	-223.39	kJ/mol	Joback Method
hf	-494.91	kJ/mol	Joback Method
hfus	22.53	kJ/mol	Joback Method
hvap	48.78	kJ/mol	Joback Method
log10ws	-2.36		Crippen Method
logp	2.595		Crippen Method
mvol	157.350	ml/mol	McGowan Method
pc	2345.09	kPa	Joback Method
rinpol	1264.00		NIST Webbook
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tb	518.60	K	Joback Method
tc	701.32	K	Joback Method
tf	278.27	K	Joback Method
vc	0.607	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	352.38	J/mol×K	518.60	Joback Method
cpg	365.50	J/mol×K	549.05	Joback Method
cpg	378.08	J/mol×K	579.51	Joback Method
cpg	390.13	J/mol×K	609.96	Joback Method
cpg	401.64	J/mol×K	640.41	Joback Method
cpg	412.64	J/mol×K	670.86	Joback Method
cpg	423.11	J/mol×K	701.32	Joback Method

dvisc	0.0040831	Paxs	278.27	Joback Method
dvisc	0.0018630	Paxs	318.32	Joback Method
dvisc	0.0010130	Paxs	358.38	Joback Method
dvisc	0.0006226	Paxs	398.44	Joback Method
dvisc	0.0004182	Paxs	438.49	Joback Method
dvisc	0.0003003	Paxs	478.55	Joback Method
dvisc	0.0002269	Paxs	518.60	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R34258&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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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