

Hexanoic acid, 3-chloroprop-2-enyl ester

Inchi:	InChI=1S/C9H15ClO2/c1-2-3-4-6-9(11)12-8-5-7-10/h5,7H,2-4,6,8H2,1H3/b7-5+
InchiKey:	SYXYWMBFAHQABF-FNORWQNLSA-N
Formula:	C9H15ClO2
SMILES:	CCCCCC(=O)OCC=CCl
Mol. weight [g/mol]:	190.67

Physical Properties

Property code	Value	Unit	Source
gf	-140.73	kJ/mol	Joback Method
hf	-372.41	kJ/mol	Joback Method
hfus	26.25	kJ/mol	Joback Method
hvap	49.13	kJ/mol	Joback Method
log10ws	-2.95		Crippen Method
logp	2.862		Crippen Method
mvol	153.050	ml/mol	McGowan Method
pc	2448.32	kPa	Joback Method
rinpol	1276.00		NIST Webbook
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tb	523.20	K	Joback Method
tc	710.07	K	Joback Method
tf	288.19	K	Joback Method
vc	0.593	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	334.06	J/molxK	523.20	Joback Method
cpg	390.36	J/molxK	678.92	Joback Method
cpg	380.17	J/molxK	647.78	Joback Method
cpg	369.46	J/molxK	616.63	Joback Method
cpg	358.22	J/molxK	585.49	Joback Method
cpg	346.42	J/molxK	554.34	Joback Method
cpg	400.04	J/molxK	710.07	Joback Method
dvisc	0.0002034	Paxs	523.20	Joback Method

dvisc	0.0002635	Paxs	484.03	Joback Method
dvisc	0.0003572	Paxs	444.86	Joback Method
dvisc	0.0005137	Paxs	405.70	Joback Method
dvisc	0.0007983	Paxs	366.53	Joback Method
dvisc	0.0013787	Paxs	327.36	Joback Method
dvisc	0.0027621	Paxs	288.19	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U299361&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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