

5-Chlorovaleric acid, 3-chloroprop-2-enyl ester

Inchi:	InChI=1S/C8H12Cl2O2/c9-5-2-1-4-8(11)12-7-3-6-10/h3,6H,1-2,4-5,7H2/b6-3+
InchiKey:	JSKLDLBTXFSIRC-ZZXXKWWIFSA-N
Formula:	C8H12Cl2O2
SMILES:	O=C(CCCCCI)OCC=CCI
Mol. weight [g/mol]:	211.09

Physical Properties

Property code	Value	Unit	Source
gf	-161.08	kJ/mol	Joback Method
hf	-367.51	kJ/mol	Joback Method
hfus	27.86	kJ/mol	Joback Method
hvap	51.29	kJ/mol	Joback Method
log10ws	-2.69		Crippen Method
logp	2.691		Crippen Method
mcvol	151.200	ml/mol	McGowan Method
pc	2597.78	kPa	Joback Method
rinsol	1484.90		NIST Webbook
tb	537.75	K	Joback Method
tc	731.85	K	Joback Method
tf	306.84	K	Joback Method
vc	0.586	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	315.65	J/molxK	537.75	Joback Method
cpg	364.54	J/molxK	699.50	Joback Method
cpg	355.78	J/molxK	667.15	Joback Method
cpg	346.53	J/molxK	634.80	Joback Method
cpg	336.77	J/molxK	602.45	Joback Method
cpg	326.48	J/molxK	570.10	Joback Method
cpg	372.83	J/molxK	731.85	Joback Method
dvisc	0.0002167	Paxs	537.75	Joback Method
dvisc	0.0002786	Paxs	499.26	Joback Method

dvisc	0.0003734	Paxs	460.78	Joback Method
dvisc	0.0005279	Paxs	422.30	Joback Method
dvisc	0.0008000	Paxs	383.81	Joback Method
dvisc	0.0013301	Paxs	345.33	Joback Method
dvisc	0.0025123	Paxs	306.84	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U292483&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

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
mccvol:	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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