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-ZZXKWVIFSA-N
Formula: C8H12Cl2O2
SMILES: O=C(CCCCCl)OC/C=C/Cl
Mol. weight [g/mol]: 211.09

Physical Properties

Property code	Value	Unit	Source
hf	-448.45	kJ/mol	Cheméo Relay (1.0)
hfus	27.86	kJ/mol	Joback Method
hvap	67.06	kJ/mol	Cheméo Relay (1.0)
ie	9.85	eV	Cheméo Relay (1.0)
logp	2.691		Crippen Method
mcvol	151.200	ml/mol	McGowan Method
rinpol	1484.90		NIST Webbook
tb	510.62	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	315.65	J/mol×K	537.75	Joback Method
cpg	326.48	J/mol×K	570.10	Joback Method
cpg	336.77	J/mol×K	602.45	Joback Method
cpg	346.53	J/mol×K	634.80	Joback Method
cpg	355.78	J/mol×K	667.15	Joback Method
cpg	364.54	J/mol×K	699.50	Joback Method
cpg	372.83	J/mol×K	731.85	Joback Method
dvisc	0.0025123	Pa×s	306.84	Joback Method
dvisc	0.0013301	Pa×s	345.33	Joback Method
dvisc	0.0008000	Pa×s	383.81	Joback Method
dvisc	0.0005279	Pa×s	422.30	Joback Method
dvisc	0.0003734	Pa×s	460.78	Joback Method
dvisc	0.0002786	Pa×s	499.26	Joback Method
dvisc	0.0002167	Pa×s	537.75	Joback Method

Sources

Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U292483&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature