Propanoic acid, 2-chloro-, 2-propenyl ester

Other names: allyl 2-chloropropionate
Inchi: InChI=1S/C6H9ClO2/c1-3-4-9-6(8)5(2)7/h3,5H,1,4H2,2H3
InchiKey: FDCTVCOKDZZPRP-UHFFFAOYSA-N
Formula: C6H9ClO2
SMILES: C=CCOC(=O)C(C)Cl
Mol. weight [g/mol]: 148.59
CAS: 55360-11-7

Physical Properties

Property code	Value	Unit	Source
gf	-160.81	kJ/mol	Joback Method
hf	-307.56	kJ/mol	Joback Method
hfus	13.48	kJ/mol	Joback Method
hvap	41.43	kJ/mol	Joback Method
log10ws	-1.32		Crippen Method
logp	1.343		Crippen Method
mcvol	110.780	ml/mol	McGowan Method
pc	3322.01	kPa	Joback Method
rinpol	904.00		NIST Webbook
rinpol	949.00		NIST Webbook
rinpol	935.00		NIST Webbook
rinpol	928.00		NIST Webbook
rinpol	914.00		NIST Webbook
ripol	1387.00		NIST Webbook
ripol	1385.00		NIST Webbook
ripol	1382.00		NIST Webbook
ripol	1385.00		NIST Webbook
tb	446.64	K	Joback Method
tc	639.20	K	Joback Method
tf	242.70	K	Joback Method
vc	0.419	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	209.02	J/mol×K	446.64	Joback Method
cpg	218.22	J/mol×K	478.73	Joback Method
cpg	227.03	J/mol×K	510.83	Joback Method
cpg	235.46	J/mol×K	542.92	Joback Method
cpg	243.52	J/mol×K	575.02	Joback Method
cpg	251.20	J/mol×K	607.11	Joback Method
cpg	258.51	J/mol×K	639.20	Joback Method
dvisc	0.0039061	Pa×s	242.70	Joback Method
dvisc	0.0019351	Pa×s	276.69	Joback Method
dvisc	0.0011179	Pa×s	310.68	Joback Method
dvisc	0.0007196	Pa×s	344.67	Joback Method
dvisc	0.0005014	Pa×s	378.66	Joback Method
dvisc	0.0003707	Pa×s	412.65	Joback Method
dvisc	0.0002870	Pa×s	446.64	Joback Method

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
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
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C55360117&Units=SI

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
ripol: Polar retention indices

tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume