Chloroacetic acid allyl ester

Other names:	Acetic acid, chloro-, 2-propenyl ester
	Acetic acid, chloro-, allyl ester
	Allyl chloroacetate
Inchi:	InChI=1S/C5H7ClO2/c1-2-3-8-5(7)4-6/h2H,1,3-4H2
InchiKey:	VMBJJCDVORDOCF-UHFFFAOYSA-N
Formula:	C5H7ClO2
SMILES:	C=CCOC(=O)CCl
Mol. weight [g/mol]:	134.56
CAS:	2916-14-5

Physical Properties

Property code	Value	Unit	Source
chl	-2603.00	kJ/mol	NIST Webbook
chl	-2606.00 ± 3.00	kJ/mol	NIST Webbook
gf	-166.79	kJ/mol	Joback Method
hf	-281.64	kJ/mol	Joback Method
hfus	14.41	kJ/mol	Joback Method
hvap	39.59	kJ/mol	Joback Method
log10ws	-0.78		Crippen Method
logp	0.954		Crippen Method
mcvol	96.690	ml/mol	McGowan Method
pc	3686.49	kPa	Joback Method
rinpol	870.00		NIST Webbook
ripol	1429.00		NIST Webbook
tb	418.20	K	NIST Webbook
tc	614.21	K	Joback Method
tf	246.43	K	Joback Method
vc	0.369	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	171.64	J/mol×K	424.20	Joback Method
cpg	206.45	J/mol×K	582.54	Joback Method

cpg	200.06	J/mol×K	550.88	Joback Method
cpg	193.40	J/mol×K	519.21	Joback Method
cpg	186.44	J/mol×K	487.54	Joback Method
cpg	179.18	J/mol×K	455.87	Joback Method
cpg	212.54	J/mol×K	614.21	Joback Method
dvisc	0.0003131	Pa×s	424.20	Joback Method
dvisc	0.0003911	Pa×s	394.57	Joback Method
dvisc	0.0005064	Pa×s	364.94	Joback Method
dvisc	0.0006863	Pa×s	335.32	Joback Method
dvisc	0.0009866	Pa×s	305.69	Joback Method
dvisc	0.0015332	Pa×s	276.06	Joback Method
dvisc	0.0026492	Pa×s	246.43	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=C2916145&Units=SI

Legend

chl: Standard liquid enthalpy of combustion
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