Allyl chloroformate

Other names:	Carbonochloridic acid, 2-propenyl ester
	Allyl chlorocarbonate
	Formic acid, chloro-, allyl ester
	Allylester kyseliny chlormravenci
	Chloroformic acid allyl ester
	UN 1722
Inchi:	InChI=1S/C4H5ClO2/c1-2-3-7-4(5)6/h2H,1,3H2
InchiKey:	CAEWJEXPFKNBQL-UHFFFAOYSA-N
Formula:	C4H5ClO2
SMILES:	C=CCOC(=O)Cl
Mol. weight [g/mol]:	120.53
CAS:	2937-50-0

Physical Properties

Property code	Value	Unit	Source
gf	-175.21	kJ/mol	Joback Method
hf	-261.00	kJ/mol	Joback Method
hfus	11.82	kJ/mol	Joback Method
hvap	37.37	kJ/mol	Joback Method
log10ws	-1.34		Crippen Method
logp	1.548		Crippen Method
mcvol	82.600	ml/mol	McGowan Method
pc	4156.97	kPa	Joback Method
tb	401.32	K	Joback Method
tc	592.92	K	Joback Method
tf	235.16	K	Joback Method
vc	0.314	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	136.77	J/mol×K	401.32	Joback Method
cpg	142.82	J/mol×K	433.25	Joback Method
cpg	148.64	J/mol×K	465.19	Joback Method

cpg	154.24	J/mol×K	497.12	Joback Method
cpg	159.61	J/mol×K	529.05	Joback Method
cpg	164.77	J/mol×K	560.99	Joback Method
cpg	169.70	J/mol×K	592.92	Joback Method
dvisc	0.0024768	Pa×s	235.16	Joback Method
dvisc	0.0014719	Pa×s	262.85	Joback Method
dvisc	0.0009660	Pa×s	290.55	Joback Method
dvisc	0.0006822	Pa×s	318.24	Joback Method
dvisc	0.0005093	Pa×s	345.93	Joback Method
dvisc	0.0003971	Pa×s	373.63	Joback Method
dvisc	0.0003204	Pa×s	401.32	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C2937500&Units=SI
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

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

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