

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	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	136.77	J/mol×K	401.32	Joback Method
cpg	164.77	J/mol×K	560.99	Joback Method
cpg	159.61	J/mol×K	529.05	Joback Method

cpg	154.24	J/molxK	497.12	Joback Method
cpg	148.64	J/molxK	465.19	Joback Method
cpg	142.82	J/molxK	433.25	Joback Method
cpg	169.70	J/molxK	592.92	Joback Method
dvisc	0.0003204	Paxs	401.32	Joback Method
dvisc	0.0003971	Paxs	373.63	Joback Method
dvisc	0.0005093	Paxs	345.93	Joback Method
dvisc	0.0006822	Paxs	318.24	Joback Method
dvisc	0.0009660	Paxs	290.55	Joback Method
dvisc	0.0014719	Paxs	262.85	Joback Method
dvisc	0.0024768	Paxs	235.16	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C2937500&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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