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

Physical Properties

Property code	Value	Unit	Source
hf	-404.96	kJ/mol	Cheméo Relay (1.0)
hfus	13.48	kJ/mol	Joback Method
hvap	46.54	kJ/mol	Cheméo Relay (1.0)
ie	10.23	eV	Cheméo Relay (1.0)
logp	1.343		Crippen Method
mcvol	110.780	ml/mol	McGowan Method
rinpol	949.00		NIST Webbook
rinpol	928.00		NIST Webbook
rinpol	935.00		NIST Webbook
rinpol	904.00		NIST Webbook
rinpol	914.00		NIST Webbook
ripol	1385.00		NIST Webbook
ripol	1385.00		NIST Webbook
ripol	1387.00		NIST Webbook
ripol	1382.00		NIST Webbook
tb	425.39	K	Cheméo Relay (1.0)

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

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C55360117&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

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
ripol: Polar retention indices
tb: Normal Boiling Point Temperature