2-Propenoic acid, 2-methyl-, 2-chloroethyl ester

Other names: «beta»-Chloroethyl methacrylate
Methacrylic acid «beta»-chloroethyl ester
Methacrylic acid, 2-chloroethyl ester
2-Chloroethyl methacrylate
Chloroethyl methacrylate
NSC 18595

Inchi: InChI=1S/C6H9ClO2/c1-5(2)6(8)9-4-3-7/h1,3-4H2,2H3

InchiKey: GPOGMJLHWQHEGF-UHFFFAOYSA-N

Formula: C6H9ClO2

SMILES: C=C(C)C(=O)OCCCl

Mol. weight [g/mol]: 148.59

CAS: 1888-94-4

Physical Properties

Property code	Value	Unit	Source
gf	-166.92	kJ/mol	Joback Method
hf	-312.07	kJ/mol	Joback Method
hfus	15.69	kJ/mol	Joback Method
hvap	41.90	kJ/mol	Joback Method
log10ws	-1.20		Crippen Method
logp	1.345		Crippen Method
mcvol	110.780	ml/mol	McGowan Method
pc	3310.55	kPa	Joback Method
tb	446.96	K	Joback Method
tc	638.85	K	Joback Method
tf	235.10 ± 0.10	K	NIST Webbook
vc	0.426	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	234.83	J/mol×K	542.90	Joback Method
cpg	242.76	J/mol×K	574.88	Joback Method
cpg	250.33	J/mol×K	606.86	Joback Method

cpg	208.81	J/mol×K	446.96	Joback Method
cpg	217.86	J/mol×K	478.94	Joback Method
cpg	226.53	J/mol×K	510.92	Joback Method
cpg	257.55	J/mol×K	638.85	Joback Method
hfust	17.00	kJ/mol	235.10	NIST Webbook
hfust	17.00	kJ/mol	235.10	NIST Webbook
sfust	72.30	J/mol×K	235.10	NIST Webbook

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=C1888944&Units=SI

Legend

cpg: Ideal gas heat capacity
gf: Standard Gibbs free energy of formation
hf: Enthalpy of formation at standard conditions
hfus: Enthalpy of fusion at standard conditions
hfust: Enthalpy of fusion at a given temperature
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
sfust: Entropy of fusion at a given temperature
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume