2-Chloroethyl methacrylate

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

Physical Properties

Property code	Value	Unit	Source
hf	-393.78	kJ/mol	Cheméo Relay (1.0)
hfus	15.69	kJ/mol	Joback Method
hvap	49.12	kJ/mol	Cheméo Relay (1.0)
ie	10.31	eV	Cheméo Relay (1.0)
log10ws	-1.57		Cheméo Relay (1.0)
logp	1.345		Crippen Method
mcvol	110.780	ml/mol	McGowan Method
tb	441.51	K	Cheméo Relay (1.0)
tf	235.10 ± 0.10	K	NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
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	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	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

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

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C1888944&Units=SI

Joback Method: https://en.wikipedia.org/wiki/Joback_method

Legend

cpg: Ideal gas heat capacity
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
ie: Ionization energy
log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
sfust: Entropy of fusion at a given temperature
tb: Normal Boiling Point Temperature
tf: Normal melting (fusion) point

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