

2-Propenoic acid, 2-chloro-, methyl ester

Other names:	Acrylic acid, 2-chloro-, methyl ester Methyl «alpha»-chloroacrylate Methyl 2-chloroacrylate 2-Chloroacrylic acid, methyl ester Methylester kyseliny 2-chlorakrylove Methyl 2-chloropropenoate Methyl 2-chloro-2-propenoate NSC 32608 Methyl alpha-chloro acrylate 2-Chloropropenoic acid, methyl ester
Inchi:	InChI=1S/C4H5ClO2/c1-3(5)4(6)7-2/h1H2,2H3
InchiKey:	AWJZTPWDQYFQPQ-UHFFFAOYSA-N
Formula:	C4H5ClO2
SMILES:	C=C(Cl)C(=O)OC
Mol. weight [g/mol]:	120.53
CAS:	80-63-7

Physical Properties

Property code	Value	Unit	Source
gf	-183.76	kJ/mol	Joback Method
hf	-270.79	kJ/mol	Joback Method
hfus	10.51	kJ/mol	Joback Method
hvap	37.45	kJ/mol	Joback Method
log10ws	-0.86		Crippen Method
logp	0.912		Crippen Method
mcvol	82.600	ml/mol	McGowan Method
pc	4183.90	kPa	Joback Method
rinpol	748.00		NIST Webbook
rinpol	766.00		NIST Webbook
ripol	1226.00		NIST Webbook
ripol	1226.00		NIST Webbook
tb	401.20	K	Joback Method
tc	596.73	K	Joback Method
tf	221.20	K	Joback Method
vc	0.315	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	136.77	J/molxK	401.20	Joback Method
cpg	142.91	J/molxK	433.79	Joback Method
cpg	148.80	J/molxK	466.38	Joback Method
cpg	154.47	J/molxK	498.97	Joback Method
cpg	159.91	J/molxK	531.55	Joback Method
cpg	165.12	J/molxK	564.14	Joback Method
cpg	170.10	J/molxK	596.73	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C80637&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
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
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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