Methyl 2-chlorobutenoate

Inchi: InChI=1S/C5H7ClO2/c1-3-4(6)5(7)8-2/h3H,1-2H3/b4-3-
InchiKey: NTMJDABWJARASG-ARJAWSKDSA-N
Formula: C5H7ClO2
SMILES: CC=C(Cl)C(=O)OC
Mol. weight [g/mol]: 134.56

Physical Properties

Property code	Value	Unit	Source
gf	-182.96	kJ/mol	Joback Method
hf	-299.64	kJ/mol	Joback Method
hfus	14.58	kJ/mol	Joback Method
hvap	40.30	kJ/mol	Joback Method
log10ws	-1.28		Crippen Method
logp	1.302		Crippen Method
mcvol	96.690	ml/mol	McGowan Method
pc	3754.57	kPa	Joback Method
rinpol	888.00		NIST Webbook
rinpol	874.00		NIST Webbook
rinpol	874.00		NIST Webbook
tb	431.56	K	Joback Method
tc	630.92	K	Joback Method
tf	229.15	K	Joback Method
vc	0.369	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	170.56	J/mol×K	431.56	Joback Method
cpg	178.48	J/mol×K	464.79	Joback Method
cpg	186.03	J/mol×K	498.01	Joback Method
cpg	193.23	J/mol×K	531.24	Joback Method
cpg	200.08	J/mol×K	564.47	Joback Method
cpg	206.60	J/mol×K	597.69	Joback Method
cpg	212.79	J/mol×K	630.92	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R80170&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

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume