E-3-Chloro-2-methyl-but-2-enal

Inchi: InChI=1S/C5H7ClO/c1-4(3-7)5(2)6/h3H,1-2H3/b5-4+
InchiKey: XFCGFNVPTTYOND-SNAWJCMRSA-N
Formula: C5H7ClO
SMILES: CC(Cl)=C(C)C=O
Mol. weight [g/mol]: 118.56

Physical Properties

Property code	Value	Unit	Source
gf	-57.11	kJ/mol	Joback Method
hf	-150.21	kJ/mol	Joback Method
hfus	12.77	kJ/mol	Joback Method
hvap	37.95	kJ/mol	Joback Method
log10ws	-1.70		Crippen Method
logp	1.718		Crippen Method
mcvol	90.820	ml/mol	McGowan Method
pc	3911.14	kPa	Joback Method
rinpol	961.90		NIST Webbook
rinpol	961.90		NIST Webbook
ripol	1383.50		NIST Webbook
tb	403.81	K	Joback Method
tc	602.25	K	Joback Method
tf	185.03	K	Joback Method
vc	0.363	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	152.80	J/mol×K	403.81	Joback Method
cpg	160.80	J/mol×K	436.88	Joback Method
cpg	168.34	J/mol×K	469.96	Joback Method
cpg	175.45	J/mol×K	503.03	Joback Method
cpg	182.14	J/mol×K	536.10	Joback Method
cpg	188.44	J/mol×K	569.18	Joback Method
cpg	194.37	J/mol×K	602.25	Joback Method

Sources

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=R153987&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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