Z-2-(1-Chloro-ethylidene)-hexanal

Inchi: InChI=1S/C7H11ClO/c1-2-3-4-7(5-8)6-9/h5-6H,2-4H2,1H3/b7-5+
InchiKey: QIDKXSZEVGNLGD-FNORWQNLSA-N
Formula: C7H11ClO
SMILES: CCCCC(C=O)=CCl
Mol. weight [g/mol]: 146.62

Physical Properties

Property code	Value	Unit	Source
gf	-31.72	kJ/mol	Joback Method
hf	-181.70	kJ/mol	Joback Method
hfus	19.26	kJ/mol	Joback Method
hvap	42.32	kJ/mol	Joback Method
log10ws	-2.53		Crippen Method
logp	2.498		Crippen Method
mcvol	119.000	ml/mol	McGowan Method
pc	3100.18	kPa	Joback Method
rinpol	1058.70		NIST Webbook
rinpol	1058.70		NIST Webbook
ripol	1492.30		NIST Webbook
ripol	1492.30		NIST Webbook
tb	449.69	K	Joback Method
tc	640.50	K	Joback Method
tf	221.53	K	Joback Method
vc	0.474	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	227.59	J/mol×K	449.69	Joback Method
cpg	238.03	J/mol×K	481.49	Joback Method
cpg	247.92	J/mol×K	513.29	Joback Method
cpg	257.29	J/mol×K	545.10	Joback Method
cpg	266.16	J/mol×K	576.90	Joback Method
cpg	274.56	J/mol×K	608.70	Joback Method

cpg	282.50	J/mol×K	640.50	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=R154108&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