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

Inchi: InChI=1S/C8H13ClO/c1-2-3-4-5-8(6-9)7-10/h6-7H,2-5H2,1H3/b8-6+
InchiKey: WGURDGMRCYHXHG-SOFGYWHQSA-N
Formula: C8H13ClO
SMILES: CCCCCC(C=O)=CCl
Mol. weight [g/mol]: 160.64

Physical Properties

Property code	Value	Unit	Source
gf	-23.30	kJ/mol	Joback Method
hf	-202.34	kJ/mol	Joback Method
hfus	21.85	kJ/mol	Joback Method
hvap	44.55	kJ/mol	Joback Method
log10ws	-2.95		Crippen Method
logp	2.888		Crippen Method
mcvol	133.090	ml/mol	McGowan Method
pc	2793.56	kPa	Joback Method
rinpol	1136.40		NIST Webbook
ripol	1590.60		NIST Webbook
ripol	1590.60		NIST Webbook
tb	472.57	K	Joback Method
tc	661.37	K	Joback Method
tf	232.80	K	Joback Method
vc	0.530	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	268.25	J/mol×K	472.57	Joback Method
cpg	279.78	J/mol×K	504.04	Joback Method
cpg	290.71	J/mol×K	535.50	Joback Method
cpg	301.08	J/mol×K	566.97	Joback Method
cpg	310.91	J/mol×K	598.44	Joback Method
cpg	320.22	J/mol×K	629.90	Joback Method
cpg	329.05	J/mol×K	661.37	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R154099&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume