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

Inchi: InChI=1S/C9H15ClO/c1-3-4-5-6-9(7-11)8(2)10/h7H,3-6H2,1-2H3/b9-8-
InchiKey: GDAAPLNTHYJTIL-HJWRWDBZSA-N
Formula: C9H15ClO
SMILES: CCCCCC(C=O)=C(C)Cl
Mol. weight [g/mol]: 174.67

Physical Properties

Property code	Value	Unit	Source
gf	-23.43	kJ/mol	Joback Method
hf	-232.77	kJ/mol	Joback Method
hfus	23.13	kJ/mol	Joback Method
hvap	46.85	kJ/mol	Joback Method
log10ws	-3.37		Crippen Method
logp	3.278		Crippen Method
mcvol	147.180	ml/mol	McGowan Method
pc	2543.05	kPa	Joback Method
rinpol	1130.10		NIST Webbook
ripol	1537.60		NIST Webbook
ripol	1537.60		NIST Webbook
tb	495.33	K	Joback Method
tc	685.47	K	Joback Method
tf	230.11	K	Joback Method
vc	0.588	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	310.82	J/mol×K	495.33	Joback Method
cpg	323.50	J/mol×K	527.02	Joback Method
cpg	335.53	J/mol×K	558.71	Joback Method
cpg	346.94	J/mol×K	590.40	Joback Method
cpg	357.76	J/mol×K	622.09	Joback Method
cpg	368.01	J/mol×K	653.78	Joback Method
cpg	377.73	J/mol×K	685.47	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R153878&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