E-3-Chloro-2-propyl-pent-2-enal

Inchi: InChI=1S/C8H13ClO/c1-3-5-7(6-10)8(9)4-2/h6H,3-5H2,1-2H3/b8-7-
InchiKey: VGVAZOMVBNUYAP-FPLPWBNLSA-N
Formula: C8H13ClO
SMILES: CCCC(C=O)=C(Cl)CC
Mol. weight [g/mol]: 160.64

Physical Properties

Property code	Value	Unit	Source
gf	-31.85	kJ/mol	Joback Method
hf	-212.13	kJ/mol	Joback Method
hfus	20.54	kJ/mol	Joback Method
hvap	44.62	kJ/mol	Joback Method
log10ws	-2.95		Crippen Method
logp	2.888		Crippen Method
mcvol	133.090	ml/mol	McGowan Method
pc	2808.38	kPa	Joback Method
rinpol	1004.40		NIST Webbook
ripol	1396.40		NIST Webbook
tb	472.45	K	Joback Method
tc	664.80	K	Joback Method
tf	218.84	K	Joback Method
vc	0.531	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	268.15	J/mol×K	472.45	Joback Method
cpg	279.86	J/mol×K	504.51	Joback Method
cpg	290.95	J/mol×K	536.57	Joback Method
cpg	301.46	J/mol×K	568.63	Joback Method
cpg	311.41	J/mol×K	600.69	Joback Method
cpg	320.83	J/mol×K	632.74	Joback Method
cpg	329.76	J/mol×K	664.80	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R154004&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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