E-3-Chloro-2-ethyl-but-2-enal

Inchi: InChI=1S/C6H9ClO/c1-3-6(4-8)5(2)7/h4H,3H2,1-2H3/b6-5-
InchiKey: REMTVJDIMSEOCW-WAYWQWQTSA-N
Formula: C6H9ClO
SMILES: CCC(C=O)=C(C)Cl
Mol. weight [g/mol]: 132.59

Physical Properties

Property code	Value	Unit	Source
gf	-48.69	kJ/mol	Joback Method
hf	-170.85	kJ/mol	Joback Method
hfus	15.36	kJ/mol	Joback Method
hvap	40.17	kJ/mol	Joback Method
log10ws	-2.12		Crippen Method
logp	2.108		Crippen Method
mcvol	104.910	ml/mol	McGowan Method
pc	3480.65	kPa	Joback Method
rinpol	954.60		NIST Webbook
rinpol	954.60		NIST Webbook
ripol	1296.30		NIST Webbook
ripol	1296.30		NIST Webbook
tb	426.69	K	Joback Method
tc	623.27	K	Joback Method
tf	196.30	K	Joback Method
vc	0.419	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	189.03	J/mol×K	426.69	Joback Method
cpg	198.41	J/mol×K	459.45	Joback Method
cpg	207.26	J/mol×K	492.22	Joback Method
cpg	215.63	J/mol×K	524.98	Joback Method
cpg	223.52	J/mol×K	557.74	Joback Method
cpg	230.97	J/mol×K	590.50	Joback Method

cpg	238.00	J/mol×K	623.27	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R153898&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

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