«alpha»-Chlorocinnamaldehyde

Other names: 2-Propenal, 2-chloro-3-phenyl-
Cinnamaldehyde, «alpha»-chloro-
Inchi: InChI=1S/C9H7ClO/c10-9(7-11)6-8-4-2-1-3-5-8/h1-7H/b9-6-
InchiKey: SARRRAKOHPKFBW-TWGQIWQCSA-N
Formula: C9H7ClO
SMILES: O=CC(Cl)=Cc1ccccc1
Mol. weight [g/mol]: 166.60
CAS: 18365-42-9

Physical Properties

Property code	Value	Unit	Source
gf	97.53	kJ/mol	Joback Method
hf	13.55	kJ/mol	Joback Method
hfus	18.49	kJ/mol	Joback Method
hvap	49.05	kJ/mol	Joback Method
log10ws	-2.64		Crippen Method
logp	2.465		Crippen Method
mcvol	123.420	ml/mol	McGowan Method
pc	3642.13	kPa	Joback Method
tb	522.13	K	Joback Method
tc	755.23	K	Joback Method
tf	270.49	K	Joback Method
vc	0.478	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	241.70	J/mol×K	522.13	Joback Method
cpg	253.02	J/mol×K	560.98	Joback Method
cpg	263.44	J/mol×K	599.83	Joback Method
cpg	273.02	J/mol×K	638.68	Joback Method
cpg	281.82	J/mol×K	677.53	Joback Method
cpg	289.92	J/mol×K	716.38	Joback Method
cpg	297.36	J/mol×K	755.23	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C18365429&Units=SI

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume