Z-(3-Chloro-2-methyl-allyloxy)-benzene

Inchi: InChI=1S/C9H9ClO/c1-8(7-10)11-9-5-3-2-4-6-9/h2-7H,1H3/b8-7-
InchiKey: MXCCQVQTIWOPFS-FPLPWBNLSA-N
Formula: C9H9ClO
SMILES: CC(=CCl)Oc1ccccc1
Mol. weight [g/mol]: 168.62

Physical Properties

Property code	Value	Unit	Source
gf	92.05	kJ/mol	Joback Method
hf	-33.09	kJ/mol	Joback Method
hfus	17.38	kJ/mol	Joback Method
hvap	44.74	kJ/mol	Joback Method
log10ws	-3.43		Crippen Method
logp	3.166		Crippen Method
mcvol	127.720	ml/mol	McGowan Method
pc	3272.78	kPa	Joback Method
rinpol	1377.70		NIST Webbook
ripol	1897.30		NIST Webbook
ripol	1897.30		NIST Webbook
tb	495.89	K	Joback Method
tc	722.51	K	Joback Method
tf	250.72	K	Joback Method
vc	0.479	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	248.08	J/mol×K	495.89	Joback Method
cpg	260.76	J/mol×K	533.66	Joback Method
cpg	272.60	J/mol×K	571.43	Joback Method
cpg	283.65	J/mol×K	609.20	Joback Method
cpg	293.94	J/mol×K	646.97	Joback Method
cpg	303.52	J/mol×K	684.74	Joback Method
cpg	312.42	J/mol×K	722.51	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=R154188&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
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