

Z-3-Chloro-2-methyl-prop-2-en-1-ol

Inchi:	InChI=1S/C4H7ClO/c1-4(2-5)3-6/h2,6H,3H2,1H3/b4-2-
InchiKey:	HIAHUGCGQSZTQU-RQOWECAXSA-N
Formula:	C4H7ClO
SMILES:	CC(=CCl)CO
Mol. weight [g/mol]:	106.55

Physical Properties

Property code	Value	Unit	Source
gf	-94.28	kJ/mol	Joback Method
hf	-186.43	kJ/mol	Joback Method
hfus	13.29	kJ/mol	Joback Method
hvap	45.60	kJ/mol	Joback Method
log10ws	-1.26		Crippen Method
logp	1.121		Crippen Method
mcvol	81.030	ml/mol	McGowan Method
pc	4504.30	kPa	Joback Method
rinpol	758.70		NIST Webbook
ripol	1566.70		NIST Webbook
tb	424.57	K	Joback Method
tc	605.66	K	Joback Method
tf	206.54	K	Joback Method
vc	0.308	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	140.67	J/mol×K	424.57	Joback Method
cpg	147.14	J/mol×K	454.75	Joback Method
cpg	153.26	J/mol×K	484.93	Joback Method
cpg	159.06	J/mol×K	515.12	Joback Method
cpg	164.55	J/mol×K	545.30	Joback Method
cpg	169.75	J/mol×K	575.48	Joback Method
cpg	174.68	J/mol×K	605.66	Joback Method

Sources

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=R154217&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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
rinpola:	Non-polar retention indices
ripola:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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