

Phenol, 2-allyl-6-chloro-

Other names:	Phenol, 2-chloro-6-[2-propenyl]-
Inchi:	InChI=1S/C9H9ClO/c1-2-4-7-5-3-6-8(10)9(7)11/h2-3,5-6,11H,1,4H2
InchiKey:	UPEBXJHGPMUFKU-UHFFFAOYSA-N
Formula:	C9H9ClO
SMILES:	C=CCc1cccc(Cl)c1O
Mol. weight [g/mol]:	168.62
CAS:	5348-07-2

Physical Properties

Property code	Value	Unit	Source
gf	48.97	kJ/mol	Joback Method
hf	-71.65	kJ/mol	Joback Method
hfus	21.42	kJ/mol	Joback Method
hvap	55.30	kJ/mol	Joback Method
log10ws	-2.78		Crippen Method
logp	2.774		Crippen Method
mcvol	127.720	ml/mol	McGowan Method
pc	3848.31	kPa	Joback Method
tb	551.71	K	Joback Method
tc	784.83	K	Joback Method
tf	370.01	K	Joback Method
vc	0.427	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	272.45	J/molxK	551.71	Joback Method
cpg	283.29	J/molxK	590.56	Joback Method
cpg	293.30	J/molxK	629.42	Joback Method
cpg	302.56	J/molxK	668.27	Joback Method
cpg	311.17	J/molxK	707.12	Joback Method
cpg	319.22	J/molxK	745.98	Joback Method
cpg	326.79	J/molxK	784.83	Joback Method
dvisc	0.0016729	Paxs	370.01	Joback Method

dvisc	0.0007757	Paxs	400.29	Joback Method
dvisc	0.0004007	Paxs	430.58	Joback Method
dvisc	0.0002258	Paxs	460.86	Joback Method
dvisc	0.0001366	Paxs	491.14	Joback Method
dvisc	0.0000875	Paxs	521.43	Joback Method
dvisc	0.0000589	Paxs	551.71	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C5348072&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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
dvisc:	Dynamic viscosity
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

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