Clorophene

Other names:	Phenol, 4-chloro-2-(phenylmethyl)-
	o-Cresol, 4-chloro-«alpha»-phenyl-
	o-Benzyl-p-chlorophenol
	p-Chloro-o-benzylphenol
	Bio-Clave
	Chlorophene
	Clorofene
	Ketolin H
	Neosabenyl
	Santophen
	Santophen 1
	Septiphene
	2-Benzyl-4-chlorophenol
	4-Chloro-«alpha»-phenyl-o-cresol
	4-Chloro-2-benzylphenol
	5-Chloro-2-hydroxydiphenylmethane
	Benzylchlorophenol
	Santophen I germicide
	NCI-C61201
	Orthobenzyl-p-chlorophenol
	Orthobenzylparachlorophenol
	Santophen 1 flake
	Santophen 1 solution
	Santophen I
	Clorophen
	2-Hydroxy-5-chlorodiphenylmethane
	Preventol BP
	Nipacide BCP
	NSC-59989
	Sentiphene
	Phenol, 4-chloro-2-benzyl-
Inchi:	InChI=1S/C13H11ClO/c14-12-6-7-13(15)11(9-12)8-10-4-2-1-3-5-10/h1-7,9,15H,8H2
InchiKey:	NCKMMSIFQUPKCK-UHFFFAOYSA-N
Formula:	C13H11ClO
SMILES:	Oc1ccc(Cl)cc1Cc1ccccc1
Mol. weight [g/mol]:	218.68
CAS:	120-32-1

Physical Properties

Property code	Value	Unit	Source
gf	107.22	kJ/mol	Joback Method
hf	-43.11	kJ/mol	Joback Method
hfus	27.10	kJ/mol	Joback Method
hvap	67.14	kJ/mol	Joback Method
log10ws	-3.81		Crippen Method
logp	3.636		Crippen Method
mcvol	164.620	ml/mol	McGowan Method
pc	3431.89	kPa	Joback Method
rinpol	1852.80		NIST Webbook
rinpol	1852.80		NIST Webbook
tb	673.23	K	Joback Method
tc	931.18	K	Joback Method
tf	443.27	K	Joback Method
vc	0.562	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	399.93	J/mol×K	673.23	Joback Method
cpg	456.78	J/mol×K	888.19	Joback Method
cpg	446.93	J/mol×K	845.20	Joback Method
cpg	436.46	J/mol×K	802.20	Joback Method
cpg	425.24	J/mol×K	759.21	Joback Method
cpg	413.11	J/mol×K	716.22	Joback Method
cpg	466.17	J/mol×K	931.18	Joback Method
dvisc	0.0000200	Pa×s	673.23	Joback Method
dvisc	0.0000292	Pa×s	634.90	Joback Method
dvisc	0.0000449	Pa×s	596.58	Joback Method
dvisc	0.0000730	Pa×s	558.25	Joback Method
dvisc	0.0001277	Pa×s	519.92	Joback Method
dvisc	0.0002442	Pa×s	481.60	Joback Method
dvisc	0.0005223	Pa×s	443.27	Joback Method

Sources

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=C120321&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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