Triclosan

Other names:	2',4',4-trichloro-2-hydroxydiphenyl ether
	2',4,4'-trichloro-2-hydroxydiphenyl ether
	2,2'-oxybis(1',5'-dichlorophenyl-5-chlorophenol)
	2,4,4'-Trichloro-2'-hydroxydiphenyl ether
	2-hydroxy-2',4,4'-trichlorodiphenyl ether
	3-chloro-6-(2,4-dichlorophenoxy)phenol
	4-chloro-2-hydroxyphenyl 2,4-dichlorophenyl ether
	5-Chloro-2-(2,4-dichlorophenoxy)phenol
	Aquasept
	CH 3565
	CH-3635
	Cloxifenolum
	DP 300
	Ether, 2'-hydroxy-2,4,4'-trichlorodiphenyl
	Gamophen
	Irgasan
	Irgasan DP300
	Phenol, 5-chloro-2-(2,4-dichlorophenoxy)-
	Phenyl ether, 2'-hydroxy-2,4,4'-trichloro-
	Sapoderm
	SterZac
	TCCP
Inchi:	InChI=1S/C12H7Cl3O2/c13-7-1-3-11(9(15)5-7)17-12-4-2-8(14)6-10(12)16/h1-6,16H
InchiKey:	XEFQLINVKFYRCS-UHFFFAOYSA-N
Formula:	C12H7Cl3O2
SMILES:	Oc1cc(Cl)ccc1Oc1ccc(Cl)cc1Cl
Mol. weight [g/mol]:	289.54
CAS:	3380-34-5

Physical Properties

Property code	Value	Unit	Source
gf	-49.32	kJ/mol	Joback Method
hf	-209.11	kJ/mol	Joback Method
hfus	33.31	kJ/mol	Joback Method
hvap	77.42	kJ/mol	Joback Method
log10ws	-4.46		Estimated Solubility Method

log10ws	-4.46		Aqueous Solubility Prediction Method
logp	5.145		Crippen Method
mcvol	180.880	ml/mol	McGowan Method
pc	3333.53	kPa	Joback Method
rinpol	2114.00		NIST Webbook
rinpol	2114.00		NIST Webbook
tb	757.59	K	Joback Method
tc	1022.29	K	Joback Method
tf	329.70	K	Aqueous Solubility Prediction Method
vc	0.623	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	411.53	J/mol×K	757.59	Joback Method
cpg	421.30	J/mol×K	801.71	Joback Method
cpg	430.36	J/mol×K	845.82	Joback Method
cpg	438.82	J/mol×K	889.94	Joback Method
cpg	446.77	J/mol×K	934.06	Joback Method
cpg	454.34	J/mol×K	978.17	Joback Method
cpg	461.64	J/mol×K	1022.29	Joback Method
dvisc	0.0001157	Pa×s	539.11	Joback Method
dvisc	0.0000682	Pa×s	575.52	Joback Method
dvisc	0.0000428	Pa×s	611.94	Joback Method
dvisc	0.0000283	Pa×s	648.35	Joback Method
dvisc	0.0000196	Pa×s	684.76	Joback Method
dvisc	0.0000141	Pa×s	721.18	Joback Method
dvisc	0.0000104	Pa×s	757.59	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C3380345&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Solubility of triclosan and iodopropynyl butylcarbamate in pure alkanols at several temperatures:	https://www.doi.org/10.1016/j.fluid.2012.05.020
Solubility of the Antimicrobial Agent Triclosan in Organic Solvents of Different Hydrogen Bonding Capabilities at Several Temperatures:	https://www.doi.org/10.1021/je800426w
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Aqueous Solubility Prediction Method: http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa

Estimated Solubility Method: http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt

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