Hexachlorophene

Other names:

Phenol, 2,2'-methylenebis[3,4,6-trichloro-
pHisoHex
Acigena
Almederm
AT-7
B 32
Bis(2-Hydroxy-3,5,6-trichlorophenyl)methane
Bis(3,5,6-trichloro-2-hydroxyphenyl)methane
Compound G-11
Cotofilm
Distodin
Exofene
Fesia-sin
Fostril
G-11
Gamophen
Gamophene
Germa-Medica
Hexabalm
Hexachlorofen
Hexachlorophen
Hexafen
Hexophene
Hexosan
Nabac
Neosept V
Ritosept
Septisol
Septofen
Steral
Steraskin
Surgi-Cen
Surofene
Tersaseptic
Trichlorophene
2,2'-Dihydroxy-3,3',5,5',6,6'-hexachlorodiphenylmethane
2,2'-Methylenebis[3,4,6-trichlorophenol]
2,2',3,3',5,5'-Hexachloro-6,6'-dihydroxydiphenylmethane
AT-17
Bis-2,3,5-trichlor-6-hydroxyfenylmethan

	Dermadex
	Fomac
	G-Eleven
	Hexachlorophane
	Hexide
	HCP
	Methane, bis(2,3,5-trichloro-6-hydroxyphenyl)
	NCI-C02653
	Phisodan
	Surgi-Cin
	Turgex
	2,2'-Dihydroxy-3,5,6,3',5',6'-hexachlorodiphenylmethane
	Bilevon
	G-II
	Isobac
	Isobac 20
	Nabac 25 EC
	RCRA Waste number U132
	UN 2875
	Bivelon
	Fascol
	Soy-Dome
	Ster-zac
	Bis[3,4,6-trichlorophenol], 2,2'-methylene-
Inchi:	InChI=1S/C13H6Cl6O2/c14-6-2-8(16)12(20)4(10(6)18)1-5-11(19)7(15)3-9(17)13(5)21/h2
InchiKey:	ACGUYXCXAPNIKK-UHFFFAOYSA-N
Formula:	C13H6Cl6O2
SMILES:	Oc1c(Cl)cc(Cl)c(Cl)c1Cc1c(O)c(Cl)cc(Cl)c1Cl
Mol. weight [g/mol]:	406.90
CAS:	70-30-4

Physical Properties

Property code	Value	Unit	Source
gf	-155.20	kJ/mol	Joback Method
hf	-356.47	kJ/mol	Joback Method
hfus	51.92	kJ/mol	Joback Method
hvap	105.39	kJ/mol	Joback Method
log10ws	-6.78		Crippen Method
logp	6.609		Crippen Method

mcvol	231.690	ml/mol	McGowan Method
pc	3025.61	kPa	Joback Method
rinpol	2807.00		NIST Webbook
rinpol	2750.00		NIST Webbook
rinpol	2807.00		NIST Webbook
rinpol	2815.00		NIST Webbook
rinpol	2750.00		NIST Webbook
tb	965.90	K	Joback Method
tc	1239.16	K	Joback Method
tf	438.14 ± 0.20	K	NIST Webbook
tf	437.00 ± 1.00	K	NIST Webbook
tf	438.20 ± 0.20	K	NIST Webbook
vc	0.773	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	522.06	J/mol×K	965.90	Joback Method
cpg	531.63	J/mol×K	1011.44	Joback Method
cpg	541.74	J/mol×K	1056.99	Joback Method
cpg	552.60	J/mol×K	1102.53	Joback Method
cpg	564.41	J/mol×K	1148.07	Joback Method
cpg	577.38	J/mol×K	1193.62	Joback Method
cpg	591.71	J/mol×K	1239.16	Joback Method
dvisc	0.0000008	Pa×s	800.31	Joback Method
dvisc	0.0000012	Pa×s	767.19	Joback Method
dvisc	0.0000006	Pa×s	833.43	Joback Method
dvisc	0.0000004	Pa×s	866.55	Joback Method
dvisc	0.0000003	Pa×s	899.66	Joback Method
dvisc	0.0000002	Pa×s	932.78	Joback Method
dvisc	0.0000002	Pa×s	965.90	Joback Method
hfust	33.26	kJ/mol	437.60	NIST Webbook
hfust	33.26	kJ/mol	437.50	NIST Webbook

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=C70304&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
hfust:	Enthalpy of fusion at a given temperature
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