Octachlorodibenzo-p-dioxin

Other names:	1,2,3,4,6,7,8,9-Octachlorodibenzo-p-dioxin
	1,2,3,4,6,7,8,9-Octachlorodibenzo[1,4]dioxin
	1,2,3,4,6,7,8,9-Octachlorodibenzodioxin
	1,2,3,4,6,7,8,9-Octachorodibenzo-p-dioxin
	Dibenzo-p-dioxin, 1,2,3,4,6,7,8,9-octachloro-
	Dibenzo-p-dioxin, octachloro-
	Dibenzo[b,e][1,4]dioxin, octachloro-
	NCI-C03678
	NSC 37651
	OCDD
	Octachloro-p-dibenzodioxin
	Octachlorodibenzo(b,e)(1,4)dioxin
	Octachlorodibenzodioxin
Inchi:	InChI=1S/C12Cl8O2/c13-1-2(14)6(18)10-9(5(1)17)21-11-7(19)3(15)4(16)8(20)12(11)22-1
InchiKey:	FOIBFBMSLDGNHL-UHFFFAOYSA-N
Formula:	C12Cl8O2
SMILES:	Clc1c(Cl)c(Cl)c2c(c1Cl)Oc1c(Cl)c(Cl)c(Cl)c(Cl)c1O2
Mol. weight [g/mol]:	459.75
CAS:	3268-87-9

Physical Properties

Property code	Value	Unit	Source
gf	-8.44	kJ/mol	Joback Method
hf	-223.27	kJ/mol	Joback Method
hfus	59.73	kJ/mol	Joback Method
hvap	97.63	kJ/mol	Joback Method
log10ws	-12.79		Aqueous Solubility Prediction Method
logp	8.812		Crippen Method
mcvol	231.220	ml/mol	McGowan Method
pc	2417.12	kPa	Joback Method
rinpol	3196.00		NIST Webbook
rinpol	3197.00		NIST Webbook
rinpol	3196.00		NIST Webbook
rinpol	3196.00		NIST Webbook
rinpol	3206.00		NIST Webbook
rinpol	3208.00		NIST Webbook

rinpol	494.40		NIST Webbook
rinpol	3196.00		NIST Webbook
rinpol	3150.00		NIST Webbook
rinpol	3197.00		NIST Webbook
rinpol	3150.00		NIST Webbook
tb	937.60	K	Joback Method
tc	1211.63	K	Joback Method
tf	721.24	K	Joback Method
vc	0.891	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	440.63	J/mol×K	937.60	Joback Method
cpg	445.68	J/mol×K	983.27	Joback Method
cpg	450.52	J/mol×K	1028.94	Joback Method
cpg	455.24	J/mol×K	1074.62	Joback Method
cpg	459.92	J/mol×K	1120.29	Joback Method
cpg	464.65	J/mol×K	1165.96	Joback Method
cpg	469.50	J/mol×K	1211.63	Joback Method
dvisc	0.0005763	Pa×s	757.30	Joback Method
dvisc	0.0006725	Pa×s	721.24	Joback Method
dvisc	0.0005009	Pa×s	793.36	Joback Method
dvisc	0.0004407	Pa×s	829.42	Joback Method
dvisc	0.0003918	Pa×s	865.48	Joback Method
dvisc	0.0003517	Pa×s	901.54	Joback Method
dvisc	0.0003183	Pa×s	937.60	Joback Method
hsubt	145.70 ± 4.00	kJ/mol	478.00	NIST Webbook
hsubt	149.80	kJ/mol	483.00	NIST Webbook

Sources

Solubilities of Selected PCDDs and PCDFs in Water and Various Chloride solutions:	https://www.doi.org/10.1021/je700185m
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C3268879&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
hsubt:	Enthalpy of sublimation 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