Dibenzo[b,E][1,4]dioxin, 2,7-dichloro-

Other names:	2,7-Dichlorodibenzo-p-dioxin
	2,7-Dichlorodibenzo[b,e] [1,4]dioxin
	2,7-Dichlorodibenzodioxin
	2,7-dichlorodibenzo-1,4-dioxin
	2,7-dichlorodibenzo[b,e][1,4]dioxin
	2,7-dichlorodioxin
	Dcdd
	Dibenzo-p-dioxin, 2,7-dichloro-
	NCI-C03667
Inchi:	InChI=1S/C12H6Cl2O2/c13-7-1-3-9-11(5-7)16-10-4-2-8(14)6-12(10)15-9/h1-6H
InchiKey:	NBFMTHWVRBOVPE-UHFFFAOYSA-N
Formula:	C12H6Cl2O2
SMILES:	Clc1ccc2c(c1)Oc1ccc(Cl)cc1O2
Mol. weight [g/mol]:	253.08
CAS:	33857-26-0

Physical Properties

Property code	Value	Unit	Source
gf	120.92	kJ/mol	Joback Method
hf	-60.01	kJ/mol	Joback Method
hfus	36.88	kJ/mol	Joback Method
hvap	67.35	kJ/mol	Joback Method
log10ws	-7.83		Aqueous Solubility Prediction Method
logp	4.891		Crippen Method
mcvol	157.780	ml/mol	McGowan Method
pc	3372.36	kPa	Joback Method
rinpol	1985.00		NIST Webbook
rinpol	1995.00		NIST Webbook
rinpol	1996.00		NIST Webbook
rinpol	1985.00		NIST Webbook
rinpol	1976.00		NIST Webbook
rinpol	1985.00		NIST Webbook
rinpol	1985.00		NIST Webbook
tb	683.14	K	Joback Method
tc	945.37	K	Joback Method

tf	474.65	K	Aqueous Solubility Prediction Method
vc	0.598	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	400.86	J/mol×K	901.66	Joback Method
cpg	407.80	J/mol×K	945.37	Joback Method
cpg	357.63	J/mol×K	683.14	Joback Method
cpg	367.82	J/mol×K	726.84	Joback Method
cpg	377.11	J/mol×K	770.55	Joback Method
cpg	385.63	J/mol×K	814.25	Joback Method
cpg	393.51	J/mol×K	857.96	Joback Method
dvisc	0.0005130	Pa×s	683.14	Joback Method
dvisc	0.0005854	Pa×s	647.05	Joback Method
dvisc	0.0015388	Pa×s	466.60	Joback Method
dvisc	0.0011999	Pa×s	502.69	Joback Method
dvisc	0.0009673	Pa×s	538.78	Joback Method
dvisc	0.0008012	Pa×s	574.87	Joback Method
dvisc	0.0006785	Pa×s	610.96	Joback Method
hsubt	105.50	kJ/mol	344.00	NIST Webbook
hsubt	113.80 ± 2.00	kJ/mol	375.50	NIST Webbook

Sources

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=C33857260&Units=SI

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Solubilities of Selected PCDDs and PCDFs in Water and Various Chloride Solutions: https://www.doi.org/10.1021/je700185m

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