Dibenzo[b,e][1,4]dioxin, 2-chloro-

Other names:	2-Chlorodibenzo-p-dioxin
	2-Chlorodibenzo-para-dioxin
	2-chloro-dibenzo[b,e][1,4]dioxin
	Dibenzo-p-dioxin, 2-chloro-
Inchi:	InChI=1S/C12H7ClO2/c13-8-5-6-11-12(7-8)15-10-4-2-1-3-9(10)14-11/h1-7H
InchiKey:	GIUGGRUEPHPVNR-UHFFFAOYSA-N
Formula:	C12H7ClO2
SMILES:	Clc1ccc2c(c1)Oc1ccccc1O2
Mol. weight [g/mol]:	218.64
CAS:	39227-54-8

Physical Properties

Property code	Value	Unit	Source
chs	-5574.80 ± 2.80	kJ/mol	NIST Webbook
gf	142.48	kJ/mol	Joback Method
hf	-74.10 ± 3.30	kJ/mol	NIST Webbook
hfs	-171.30 ± 3.20	kJ/mol	NIST Webbook
hfus	33.07	kJ/mol	Joback Method
hsub	97.24 ± 0.55	kJ/mol	NIST Webbook
hsub	97.20 ± 0.60	kJ/mol	NIST Webbook
hsub	97.20	kJ/mol	NIST Webbook
hsub	98.10 ± 1.10	kJ/mol	NIST Webbook
hvap	62.30	kJ/mol	Joback Method
ie	7.71 ± 0.00	eV	NIST Webbook
log10ws	-5.87		Aqueous Solubility Prediction Method
logp	4.238		Crippen Method
mcvol	145.540	ml/mol	McGowan Method
pc	3585.64	kPa	Joback Method
rinpol	1825.00		NIST Webbook
rinpol	1826.00		NIST Webbook
tb	640.73	K	Joback Method
tc	899.71	K	Joback Method
tf	362.00 ± 0.10	K	NIST Webbook
vc	0.548	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	386.98	J/mol×K	856.54	Joback Method
cpg	394.59	J/mol×K	899.71	Joback Method
cpg	338.40	J/mol×K	640.73	Joback Method
cpg	349.94	J/mol×K	683.89	Joback Method
cpg	360.45	J/mol×K	727.06	Joback Method
cpg	370.04	J/mol×K	770.22	Joback Method
cpg	378.84	J/mol×K	813.38	Joback Method
dvisc	0.0005249	Pa×s	640.73	Joback Method
dvisc	0.0006035	Pa×s	604.63	Joback Method
dvisc	0.0017305	Pa×s	424.16	Joback Method
dvisc	0.0013121	Pa×s	460.25	Joback Method
dvisc	0.0010357	Pa×s	496.35	Joback Method
dvisc	0.0008442	Pa×s	532.45	Joback Method
dvisc	0.0007062	Pa×s	568.54	Joback Method
hfust	23.10	kJ/mol	362.20	NIST Webbook
hsubt	97.20	kJ/mol	326.50	NIST Webbook

Sources

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

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=C39227548&Units=SI

Legend

chs: Standard solid enthalpy of combustion

cpg: Ideal gas heat capacity

dvisc: Dynamic viscosity

gf: Standard Gibbs free energy of formation

hf: Enthalpy of formation at standard conditions

hfs:	Solid phase enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hfust:	Enthalpy of fusion at a given temperature
hsub:	Enthalpy of sublimation at standard conditions
hsubt:	Enthalpy of sublimation at a given temperature
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
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