Dibenzo-p-dioxin

Other names:	Dibenzo[1,4]dioxin
	Dibenzo[b,e][1,4]dioxin
	Dibenzodioxin
	Diphenylene dioxide
	NCI-C03656
	Oxanthrene
	Phenodioxin
	dibenzo-p-dioxine
Inchi:	InChI=1S/C12H8O2/c1-2-6-10-9(5-1)13-11-7-3-4-8-12(11)14-10/h1-8H
InchiKey:	NFBOHOGPQUYFRF-UHFFFAOYSA-N
Formula:	C12H8O2
SMILES:	c1ccc2c(c1)Oc1ccccc1O2
Mol. weight [g/mol]:	184.19
CAS:	262-12-4

Physical Properties

Property code	Value	Unit	Source
chs	-5716.70 ± 4.10	kJ/mol	NIST Webbook
chs	-5716.70 ± 4.10	kJ/mol	NIST Webbook
gf	164.04	kJ/mol	Joback Method
hf	-59.20	kJ/mol	NIST Webbook
hf	-59.20 ± 4.40	kJ/mol	NIST Webbook
hf	-59.20 ± 4.40	kJ/mol	NIST Webbook
hfs	-148.70 ± 4.40	kJ/mol	NIST Webbook
hfs	-148.70 ± 4.40	kJ/mol	NIST Webbook
hfus	29.26	kJ/mol	Joback Method
hsub	89.60 ± 0.70	kJ/mol	NIST Webbook
hsub	91.50 ± 0.80	kJ/mol	NIST Webbook
hsub	89.50	kJ/mol	NIST Webbook
hvap	57.25	kJ/mol	Joback Method
ie	8.10 ± 0.03	eV	NIST Webbook
ie	7.60 ± 0.00	eV	NIST Webbook
ie	7.60 ± 0.00	eV	NIST Webbook
ie	7.70	eV	NIST Webbook
ie	7.78 ± 0.05	eV	NIST Webbook
ie	7.50	eV	NIST Webbook

log10ws	-5.32		Aqueous Solubility Prediction Method
logp	3.585		Crippen Method
mcvol	133.300	ml/mol	McGowan Method
pc	3819.82	kPa	Joback Method
rinpol	1612.00		NIST Webbook
rinpol	267.27		NIST Webbook
rinpol	1612.00		NIST Webbook
tb	598.32	K	Joback Method
tc	853.36	K	Joback Method
tf	395.40	K	Aqueous Solubility Prediction Method
tf	395.70 ± 0.10	K	NIST Webbook
tf	393.05 ± 0.50	K	NIST Webbook
vc	0.499	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	341.92	J/mol×K	683.33	Joback Method
cpg	380.10	J/mol×K	853.36	Joback Method
cpg	371.70	J/mol×K	810.85	Joback Method
cpg	362.62	J/mol×K	768.34	Joback Method
cpg	352.73	J/mol×K	725.84	Joback Method
cpg	316.99	J/mol×K	598.32	Joback Method
cpg	330.04	J/mol×K	640.83	Joback Method
dvisc	0.0010845	Pa×s	453.92	Joback Method
dvisc	0.0008673	Pa×s	490.02	Joback Method
dvisc	0.0007152	Pa×s	526.12	Joback Method
dvisc	0.0006046	Pa×s	562.22	Joback Method
dvisc	0.0005215	Pa×s	598.32	Joback Method
dvisc	0.0019248	Pa×s	381.72	Joback Method
dvisc	0.0014094	Pa×s	417.82	Joback Method
hfust	23.20	kJ/mol	395.70	NIST Webbook
hsubt	92.30	kJ/mol	318.00	NIST Webbook
hsubt	89.60 ± 0.70	kJ/mol	318.00	NIST Webbook
hsubt	89.55	kJ/mol	318.00	NIST Webbook
hsubt	89.55 ± 0.72	kJ/mol	318.00	NIST Webbook
hsubt	93.60 ± 1.20	kJ/mol	318.00	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=C262124&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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