1,3,6,8-Tetrachlorodibenzo-p-dioxin

Other names:	1,3,6,8-TCDD
	1,3,6,8-Tetrachlorobenzo-p-dioxin
	1,3,6,8-Tetrachlorodibenzo-para-dioxin
	1,3,6,8-Tetrachlorodibenzo[1,4]dioxin
	1,3,6,8-Tetrachlorodibenzo[b,e] [1,4]dioxin
	1,3,6,8-Tetrachlorodibenzodioxin
	1,3,6,8-Tetrachlorooxanthrene
	Dibenzo(b,e)(1,4)dioxin, 1,3,6,8-tetrachloro-
	Dibenzo-p-dioxin, 1,3,6,8-tetrachloro-
Inchi:	InChI=1S/C12H4Cl4O2/c13-5-1-7(15)11-9(3-5)18-12-8(16)2-6(14)4-10(12)17-11/h1-4H
InchiKey:	OTQFXRBLGNEOGH-UHFFFAOYSA-N
Formula:	C12H4Cl4O2
SMILES:	Clc1cc(Cl)c2c(c1)Oc1c(Cl)cc(Cl)cc1O2
Mol. weight [g/mol]:	321.97
CAS:	33423-92-6

Physical Properties

Property code	Value	Unit	Source
gf	77.80	kJ/mol	Joback Method
hf	-114.43	kJ/mol	Joback Method
hfus	44.49	kJ/mol	Joback Method
hvap	77.44	kJ/mol	Joback Method
log10ws	-9.00		Aqueous Solubility Prediction Method
logp	6.198		Crippen Method
mcvol	182.260	ml/mol	McGowan Method
pc	2999.15	kPa	Joback Method
rinpol	2260.00		NIST Webbook
rinpol	2260.00		NIST Webbook
rinpol	2260.00		NIST Webbook
rinpol	2260.00		NIST Webbook
rinpol	2290.00		NIST Webbook
rinpol	2262.00		NIST Webbook
rinpol	2290.00		NIST Webbook
rinpol	2290.00		NIST Webbook
rinpol	2290.00		NIST Webbook
rinpol	2262.00		NIST Webbook

rinpol	2260.00		NIST Webbook
rinpol	2290.00		NIST Webbook
tb	767.96	K	Joback Method
tc	1035.13	K	Joback Method
tf	551.48	K	Joback Method
vc	0.696	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	431.25	J/mol×K	1035.13	Joback Method
cpg	390.63	J/mol×K	767.96	Joback Method
cpg	398.57	J/mol×K	812.49	Joback Method
cpg	405.89	J/mol×K	857.02	Joback Method
cpg	412.71	J/mol×K	901.55	Joback Method
cpg	419.14	J/mol×K	946.08	Joback Method
cpg	425.28	J/mol×K	990.60	Joback Method
dvisc	0.0004605	Pa×s	767.96	Joback Method
dvisc	0.0011898	Pa×s	551.48	Joback Method
dvisc	0.0009675	Pa×s	587.56	Joback Method
dvisc	0.0008058	Pa×s	623.64	Joback Method
dvisc	0.0006847	Pa×s	659.72	Joback Method
dvisc	0.0005917	Pa×s	695.80	Joback Method
dvisc	0.0005188	Pa×s	731.88	Joback Method
hsubt	118.60 ± 3.20	kJ/mol	393.00	NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C33423926&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Joback Method: https://en.wikipedia.org/wiki/Joback_method
Aqueous Solubility Prediction Method: http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa

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