Dibenzo-p-dioxin, 1,2,3,4,6,9-hexachloro

Other names: 1,2,3,4,6,9-hexachlorodibenzo-p-dioxin
1,2,3,4,6,9-hexachlorodibenzo[b,e][1,4]dioxin
1,2,3,4,6,9-hexachlorodibenzodioxin
dibenzo[b,e][1,4]dioxin, 1,2,3,4,6,9-hexachloro-
Inchi: InChI=1S/C12H2Cl6O2/c13-3-1-2-4(14)10-9(3)19-11-7(17)5(15)6(16)8(18)12(11)20-10/h
InchiKey: UDYXCMRDCOVQLG-UHFFFAOYSA-N
Formula: C12H2Cl6O2
SMILES: Clc1ccc(Cl)c2c1Oc1c(Cl)c(Cl)c(Cl)c(Cl)c1O2
Mol. weight [g/mol]: 390.86

Physical Properties

Property code	Value	Unit	Source
gf	34.68	kJ/mol	Joback Method
hf	-168.85	kJ/mol	Joback Method
hfus	52.11	kJ/mol	Joback Method
hvap	87.53	kJ/mol	Joback Method
log10ws	-7.10		Crippen Method
logp	7.505		Crippen Method
mcvol	206.740	ml/mol	McGowan Method
pc	2684.64	kPa	Joback Method
rinpol	2769.00		NIST Webbook
rinpol	2769.00		NIST Webbook
rinpol	2751.00		NIST Webbook
rinpol	2752.00		NIST Webbook
tb	852.78	K	Joback Method
tc	1123.61	K	Joback Method
tf	636.36	K	Joback Method
vc	0.793	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	417.83	J/mol×K	852.78	Joback Method
cpg	424.09	J/mol×K	897.92	Joback Method

cpg	429.98	J/mol×K	943.06	Joback Method
cpg	435.58	J/mol×K	988.19	Joback Method
cpg	440.99	J/mol×K	1033.33	Joback Method
cpg	446.32	J/mol×K	1078.47	Joback Method
cpg	451.65	J/mol×K	1123.61	Joback Method
dvisc	0.0009011	Pa×s	636.36	Joback Method
dvisc	0.0007551	Pa×s	672.43	Joback Method
dvisc	0.0006442	Pa×s	708.50	Joback Method
dvisc	0.0005581	Pa×s	744.57	Joback Method
dvisc	0.0004900	Pa×s	780.64	Joback Method
dvisc	0.0004352	Pa×s	816.71	Joback Method
dvisc	0.0003904	Pa×s	852.78	Joback Method

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R50024&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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
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