1,2,3,6,7-pentachloro dibenzo-p-dioxin

Other names: Dibenzo-p-dioxin, 1,2,3,6,7-pentachloro
Inchi: InChI=1S/C12H3Cl5O2/c13-4-1-2-6-11(9(4)16)19-7-3-5(14)8(15)10(17)12(7)18-6/h1-3H
InchiKey: RLGWDUHOIIWPGN-UHFFFAOYSA-N
Formula: C12H3Cl5O2
SMILES: Clc1cc2c(c(Cl)c1Cl)Oc1ccc(Cl)c(Cl)c1O2
Mol. weight [g/mol]: 356.42

Physical Properties

Property code	Value	Unit	Source
gf	56.24	kJ/mol	Joback Method
hf	-141.64	kJ/mol	Joback Method
hfus	48.30	kJ/mol	Joback Method
hvap	82.49	kJ/mol	Joback Method
log10ws	-6.41		Crippen Method
logp	6.852		Crippen Method
mcvol	194.500	ml/mol	McGowan Method
pc	2835.36	kPa	Joback Method
rinpol	2604.00		NIST Webbook
rinpol	2598.00		NIST Webbook
rinpol	2604.00		NIST Webbook
rinpol	2569.00		NIST Webbook
rinpol	2569.00		NIST Webbook
rinpol	2604.00		NIST Webbook
rinpol	2598.00		NIST Webbook
rinpol	2569.00		NIST Webbook
rinpol	2604.00		NIST Webbook
tb	810.37	K	Joback Method
tc	1079.48	K	Joback Method
tf	593.92	K	Joback Method
vc	0.745	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source

cpg	404.85	J/mol×K	810.37	Joback Method
cpg	436.17	J/mol×K	1034.63	Joback Method
cpg	430.47	J/mol×K	989.77	Joback Method
cpg	424.59	J/mol×K	944.92	Joback Method
cpg	418.44	J/mol×K	900.07	Joback Method
cpg	411.89	J/mol×K	855.22	Joback Method
cpg	441.79	J/mol×K	1079.48	Joback Method
dvisc	0.0004264	Pa×s	810.37	Joback Method
dvisc	0.0004778	Pa×s	774.30	Joback Method
dvisc	0.0005413	Pa×s	738.22	Joback Method
dvisc	0.0006211	Pa×s	702.14	Joback Method
dvisc	0.0007235	Pa×s	666.07	Joback Method
dvisc	0.0008575	Pa×s	630.00	Joback Method
dvisc	0.0010376	Pa×s	593.92	Joback Method

Sources

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

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

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=R37428&Units=SI

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