1,2,4,7,8-PENTACHLORODIBENZO-P-DIOXIN

Other names: Dibenzo-p-dioxin, 1,2,4,7,8-pentachloro-
1,2,4,7,8-Pentachlorodibenzo[b,e] [1,4]dioxin
Inchi: InChI=1S/C12H3Cl5O2/c13-4-2-8-9(3-5(4)14)19-12-10(17)6(15)1-7(16)11(12)18-8/h1-3H
InchiKey: QUPLGUUISJOUPJ-UHFFFAOYSA-N
Formula: C12H3Cl5O2
SMILES: Clc1cc2c(cc1Cl)Oc1c(Cl)c(Cl)cc(Cl)c1O2
Mol. weight [g/mol]: 356.42

Physical Properties

Property code	Value	Unit	Source
hfus	48.30	kJ/mol	Joback Method
log10ws	-9.73		Cheméo Relay (1.0)
logp	6.852		Crippen Method
mcvol	194.500	ml/mol	McGowan Method
rinpol	2545.00		NIST Webbook
rinpol	2554.00		NIST Webbook
rinpol	2555.00		NIST Webbook
rinpol	2554.00		NIST Webbook
rinpol	2545.00		NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	404.85	J/mol×K	810.37	Joback Method
cpg	411.89	J/mol×K	855.22	Joback Method
cpg	418.44	J/mol×K	900.07	Joback Method
cpg	424.59	J/mol×K	944.92	Joback Method
cpg	430.47	J/mol×K	989.77	Joback Method
cpg	436.17	J/mol×K	1034.63	Joback Method
cpg	441.79	J/mol×K	1079.48	Joback Method
dvisc	0.0010376	Pa×s	593.92	Joback Method
dvisc	0.0008575	Pa×s	630.00	Joback Method
dvisc	0.0007235	Pa×s	666.07	Joback Method
dvisc	0.0006211	Pa×s	702.14	Joback Method

dvisc	0.0005413	Pa×s	738.22	Joback Method
dvisc	0.0004778	Pa×s	774.30	Joback Method
dvisc	0.0004264	Pa×s	810.37	Joback Method
hsubt	125.30 ± 2.30	kJ/mol	415.50	NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C58802087&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
hfus:	Enthalpy of fusion at standard conditions
hsubt:	Enthalpy of sublimation at a given temperature
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices