

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
CAS:	58802-08-7

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	2555.00		NIST Webbook
rinpol	2554.00		NIST Webbook
rinpol	2545.00		NIST Webbook
rinpol	2554.00		NIST Webbook
rinpol	2545.00		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	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

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C58802087&Units=SI
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

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

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