

1,2,3,7,8-Pentachlorodibenzodioxin

Other names:

Dibenzo-p-dioxin, 1,2,3,7,8-pentachloro-
1,2,3,7,8-Pentachlorodibenzo-p-dioxin
1,2,3,7,8-Penta polychlorinated dibenzo-p-dioxin

Inchi: InChI=1S/C12H3Cl5O2/c13-4-1-7-8(2-5(4)14)19-12-9(18-7)3-6(15)10(16)11(12)17/h1-3H**InchiKey:** FSPZPQQWDODWAU-UHFFFAOYSA-N**Formula:** C12H3Cl5O2**SMILES:** Clc1cc2c(cc1Cl)Oc1c(cc(Cl)c(Cl)c1Cl)O2**Mol. weight [g/mol]:** 356.42**CAS:** 40321-76-4

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	2587.00		NIST Webbook
rinpol	2587.00		NIST Webbook
rinpol	2581.00		NIST Webbook
rinpol	2574.00		NIST Webbook
rinpol	2581.00		NIST Webbook
rinpol	2555.00		NIST Webbook
rinpol	2587.00		NIST Webbook
rinpol	2587.00		NIST Webbook
tb	810.37	K	Joback Method
tc	1079.48	K	Joback Method
tf	593.92	K	Joback Method
vc	0.745	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	404.85	J/molxK	810.37	Joback Method
cpg	411.89	J/molxK	855.22	Joback Method
cpg	418.44	J/molxK	900.07	Joback Method
cpg	424.59	J/molxK	944.92	Joback Method
cpg	430.47	J/molxK	989.77	Joback Method
cpg	436.17	J/molxK	1034.63	Joback Method
cpg	441.79	J/molxK	1079.48	Joback Method
dvisc	0.0010376	Paxs	593.92	Joback Method
dvisc	0.0008575	Paxs	630.00	Joback Method
dvisc	0.0007235	Paxs	666.07	Joback Method
dvisc	0.0006211	Paxs	702.14	Joback Method
dvisc	0.0005413	Paxs	738.22	Joback Method
dvisc	0.0004778	Paxs	774.30	Joback Method
dvisc	0.0004264	Paxs	810.37	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C40321764&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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

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