Dibenzo-p-dioxin, 1,2,3,4,7-pentachloro-

Other names: 1,2,3,4,7-pentachloro dibenzo-p-dioxin
Inchi: InChI=1S/C12H3Cl5O2/c13-4-1-2-5-6(3-4)19-12-10(17)8(15)7(14)9(16)11(12)18-5/h1-3H
InchiKey: WRNGAZFESPEMCN-UHFFFAOYSA-N
Formula: C12H3Cl5O2
SMILES: Clc1ccc2c(c1)Oc1c(Cl)c(Cl)c(Cl)c(Cl)c1O2
Mol. weight [g/mol]: 356.42
CAS: 39227-61-7

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	2573.00		NIST Webbook
rinpol	2583.00		NIST Webbook
rinpol	2582.00		NIST Webbook
rinpol	2573.00		NIST Webbook
rinpol	2573.00		NIST Webbook
rinpol	2576.00		NIST Webbook
rinpol	2573.00		NIST Webbook
rinpol	2576.00		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

Sources

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=C39227617&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