Dibenzo-p-dioxin, 1,2,3,4,6-pentachloro

Inchi: InChI=1S/C12H3Cl5O2/c13-4-2-1-3-5-10(4)19-12-9(17)7(15)6(14)8(16)11(12)18-5/h1-3H
InchiKey: LNWDBNKKBLRAMH-UHFFFAOYSA-N
Formula: C12H3Cl5O2
SMILES: Clc1cccc2c1Oc1c(Cl)c(Cl)c(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	2573.00		NIST Webbook
rinpol	2586.00		NIST Webbook
rinpol	2573.00		NIST Webbook
rinpol	2573.00		NIST Webbook
rinpol	2586.00		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

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=R50038&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

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