Dibenzo-p-dioxin, 1,2,4,8,9-pentachloro

Inchi: InChI=1S/C12H3Cl5O2/c13-4-1-2-7-11(8(4)16)19-12-9(17)5(14)3-6(15)10(12)18-7/h1-3H
InchiKey: KLLFLRKEOJCTGC-UHFFFAOYSA-N
Formula: C12H3Cl5O2
SMILES: Clc1ccc2c(c1Cl)Oc1c(Cl)c(Cl)cc(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	2545.00		NIST Webbook
rinpol	2570.00		NIST Webbook
rinpol	2545.00		NIST Webbook
rinpol	2570.00		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

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=R50177&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