Dibenzo-p-dioxin, 1,2,3,4,6,7,9-heptachloro-

Other names:	1,2,3,4,6,7,9-Heptachlorodibenzodioxin
	1,2,3,4,6,7,9-Heptachlorodibenzo[b,e] [1,4]dioxin
Inchi:	InChI=1S/C12HCl7O2/c13-2-1-3(14)9-10(4(2)15)21-12-8(19)6(17)5(16)7(18)11(12)20-9/h
InchiKey:	KTJJIBIRZGQFQZ-UHFFFAOYSA-N
Formula:	C12HCl7O2
SMILES:	Clc1cc(Cl)c2c(c1Cl)Oc1c(Cl)c(Cl)c(Cl)c(Cl)c1O2
Mol. weight [g/mol]:	425.31
CAS:	58200-70-7

Physical Properties

Property code	Value	Unit	Source
gf	13.12	kJ/mol	Joback Method
hf	-196.06	kJ/mol	Joback Method
hfus	55.92	kJ/mol	Joback Method
hvap	92.58	kJ/mol	Joback Method
log10ws	-7.78		Crippen Method
logp	8.158		Crippen Method
mcvol	218.980	ml/mol	McGowan Method
pc	2545.61	kPa	Joback Method
rinpol	464.45		NIST Webbook
rinpol	2949.00		NIST Webbook
rinpol	2961.00		NIST Webbook
tb	895.19	K	Joback Method
tc	1167.63	K	Joback Method
tf	678.80	K	Joback Method
vc	0.843	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	429.71	J/mol×K	895.19	Joback Method
cpg	455.80	J/mol×K	1122.22	Joback Method
cpg	450.79	J/mol×K	1076.81	Joback Method
cpg	445.77	J/mol×K	1031.41	Joback Method

cpg	440.64	J/mol×K	986.00	Joback Method
cpg	435.32	J/mol×K	940.60	Joback Method
cpg	460.89	J/mol×K	1167.63	Joback Method
dvisc	0.0003540	Pa×s	895.19	Joback Method
dvisc	0.0003928	Pa×s	859.12	Joback Method
dvisc	0.0004398	Pa×s	823.06	Joback Method
dvisc	0.0004976	Pa×s	787.00	Joback Method
dvisc	0.0005697	Pa×s	750.93	Joback Method
dvisc	0.0006612	Pa×s	714.87	Joback Method
dvisc	0.0007797	Pa×s	678.80	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C58200707&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
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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