1,2,3,4,6,7,8-Heptachlorodibenzodioxin

Other names: 1,2,3,4,6,7,8-heptachlorodibenzo-p-dioxin
Dibenzo-p-dioxin, 1,2,3,4,6,7,8-heptachloro
Inchi: InChI=1S/C12HCl7O2/c13-2-1-3-10(7(17)4(2)14)21-12-9(19)6(16)5(15)8(18)11(12)20-3/h
InchiKey: WCLNVRQZUKYVAI-UHFFFAOYSA-N
Formula: C12HCl7O2
SMILES: Clc1cc2c(c(Cl)c1Cl)Oc1c(Cl)c(Cl)c(Cl)c(Cl)c1O2
Mol. weight [g/mol]: 425.31
CAS: 35822-46-9

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	-11.25		Aqueous Solubility Prediction Method
logp	8.158		Crippen Method
mcvol	218.980	ml/mol	McGowan Method
pc	2545.61	kPa	Joback Method
rinpol	2971.00		NIST Webbook
rinpol	2994.00		NIST Webbook
rinpol	470.46		NIST Webbook
rinpol	2994.00		NIST Webbook
rinpol	2996.00		NIST Webbook
rinpol	2994.00		NIST Webbook
rinpol	2992.00		NIST Webbook
rinpol	2993.00		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

Aqueous Solubility Prediction Method: http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C35822469&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
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