1,2,3,6,7,8-Hexachlorodibenzo-p-dioxin

Other names: Dibenzo-p-dioxin, 1,2,3,6,7,8-hexachloro-
Dibenzo(b,e)(1,4)dioxin, 1,2,3,6,7,8-hexachloro-
1,2,3,6,7,8-Hexachloro-p-dioxin
1,2,3,6,7,8-Hexachlorodibenzodioxin
Inchi: InChI=1S/C12H2Cl6O2/c13-3-1-5-11(9(17)7(3)15)20-6-2-4(14)8(16)10(18)12(6)19-5/h1-2
InchiKey: YCLUIPQDHHPDJJ-UHFFFAOYSA-N
Formula: C12H2Cl6O2
SMILES: Clc1cc2c(c(Cl)c1Cl)Oc1cc(Cl)c(Cl)c(Cl)c1O2
Mol. weight [g/mol]: 390.86
CAS: 57653-85-7

Physical Properties

Property code	Value	Unit	Source
gf	34.68	kJ/mol	Joback Method
hf	-168.85	kJ/mol	Joback Method
hfus	52.11	kJ/mol	Joback Method
hvap	87.53	kJ/mol	Joback Method
log10ws	-7.10		Crippen Method
logp	7.505		Crippen Method
mcvol	206.740	ml/mol	McGowan Method
pc	2684.64	kPa	Joback Method
rinpol	2788.00		NIST Webbook
rinpol	2788.00		NIST Webbook
rinpol	2749.00		NIST Webbook
rinpol	2782.00		NIST Webbook
rinpol	2749.00		NIST Webbook
rinpol	2788.00		NIST Webbook
rinpol	2788.00		NIST Webbook
rinpol	2788.00		NIST Webbook
rinpol	2747.00		NIST Webbook
rinpol	2782.00		NIST Webbook
rinpol	2782.00		NIST Webbook
tb	852.78	K	Joback Method
tc	1123.61	K	Joback Method
tf	636.36	K	Joback Method
vc	0.793	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	417.83	J/mol×K	852.78	Joback Method
cpg	424.09	J/mol×K	897.92	Joback Method
cpg	429.98	J/mol×K	943.06	Joback Method
cpg	435.58	J/mol×K	988.19	Joback Method
cpg	440.99	J/mol×K	1033.33	Joback Method
cpg	446.32	J/mol×K	1078.47	Joback Method
cpg	451.65	J/mol×K	1123.61	Joback Method
dvisc	0.0009011	Pa×s	636.36	Joback Method
dvisc	0.0007551	Pa×s	672.43	Joback Method
dvisc	0.0006442	Pa×s	708.50	Joback Method
dvisc	0.0005581	Pa×s	744.57	Joback Method
dvisc	0.0004900	Pa×s	780.64	Joback Method
dvisc	0.0004352	Pa×s	816.71	Joback Method
dvisc	0.0003904	Pa×s	852.78	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=C57653857&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