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

Physical Properties

Property code	Value	Unit	Source
hf	-148.14	kJ/mol	Cheméo Relay (1.0)
hfus	52.11	kJ/mol	Joback Method
hvap	111.80	kJ/mol	Cheméo Relay (1.0)
ie	8.21	eV	Cheméo Relay (1.0)
log10ws	-10.73		Cheméo Relay (1.0)
logp	7.505		Crippen Method
mcvol	206.740	ml/mol	McGowan Method
rinpol	2788.00		NIST Webbook
rinpol	2782.00		NIST Webbook
rinpol	2788.00		NIST Webbook
rinpol	2749.00		NIST Webbook
rinpol	2782.00		NIST Webbook
rinpol	2788.00		NIST Webbook
rinpol	2782.00		NIST Webbook
rinpol	2788.00		NIST Webbook
rinpol	2747.00		NIST Webbook
rinpol	2788.00		NIST Webbook
rinpol	2749.00		NIST Webbook
tb	647.88	K	Cheméo Relay (1.0)
tf	516.31	K	Cheméo Relay (1.0)

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

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C57653857&Units=SI

Joback Method: https://en.wikipedia.org/wiki/Joback_method

Legend

cpg: Ideal gas heat capacity

dvisc: Dynamic viscosity

hf: Enthalpy of formation at standard conditions

hfus: Enthalpy of fusion at standard conditions

hvap: Enthalpy of vaporization at standard conditions

ie: Ionization energy

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point