Bi-2,4-cyclopentadien-1-yl, 1,1',2,2',3,3',4,4',5,5'-decachloro-

Other names: 1,1',2,2',3,3',4,4',5,5'-Decachlorobi-2,4-cyclopentadien-1-yl
1,2,3,4,5-pentachloro-5-(1,2,3,4,5-pentachloro-1-cyclopenta-2,4-dienyl)cyclopenta-1,3-die
Bi-2,4-cyclopentadien-1-yl, decachloro-
Bis(pentachlor-2,4-cyclopentadien-1-yl)
Bis(pentachloro-2,4-cyclopentadien-1-yl)
Bis(pentachlorocyclopentadienyl)
Decachlor
Decachlorobi-2,4-cyclopentadien-1-yl
Decachlorobi-2,4-cyclopentadiene-1-yl
Decachlorobis(2,4-cyclopentadiene-1-yl)
Dienochlor
Dienochlore
ENT 25,718
HRS 16
HRS 1654
HRS 16A
Hooker HRS 1654
Hooker HRS-16
NSC 26106
NSC 41880
Pentac
Pentac SP
Pentac WP
Pentac aquaflow

Inchi: InChI=1S/C10Cl10/c11-1-2(12)6(16)9(19,5(1)15)10(20)7(17)3(13)4(14)8(10)18

InchiKey: LWLJUMBEZJHXHV-UHFFFAOYSA-N

Formula: C10Cl10

SMILES: ClC1=C(Cl)C(Cl)(C2(Cl)C(Cl)=C(Cl)C(Cl)=C2Cl)C(Cl)=C1Cl

Mol. weight [g/mol]: 474.64

Physical Properties

Property code	Value	Unit	Source
hf	42.16	kJ/mol	Cheméo Relay (1.0)
hfus	40.68	kJ/mol	Joback Method
hvap	100.53	kJ/mol	Cheméo Relay (1.0)
log10ws	-7.28		Aqueous Solubility Prediction Method

log10ws	-7.28		Estimated Solubility Method
logp	7.726		Crippen Method
mcvol	235.240	ml/mol	McGowan Method
tb	589.31	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	416.13	J/mol×K	870.02	Joback Method
cpg	426.64	J/mol×K	917.86	Joback Method
cpg	439.17	J/mol×K	965.69	Joback Method
cpg	454.20	J/mol×K	1013.53	Joback Method
cpg	472.16	J/mol×K	1061.37	Joback Method
cpg	493.52	J/mol×K	1109.21	Joback Method
cpg	518.72	J/mol×K	1157.04	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C2227170&Units=SI
Joback Method: https://en.wikipedia.org/wiki/Joback_method
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Cheméo Relay (1.0):
Cheméo Relay (1.0, beta):
Aqueous Solubility Prediction Method: http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
Estimated Solubility Method: http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt

Legend

cpg: Ideal gas heat capacity
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
tb:	Normal Boiling Point Temperature