

2,2',4,4',5,5'-Hexachlorodiphenyl ether

Inchi:	InChI=1S/C12H4Cl6O/c13-5-1-9(17)11(3-7(5)15)19-12-4-8(16)6(14)2-10(12)18/h1-4H
InchiKey:	PECXRRMHOQBOIE-UHFFFAOYSA-N
Formula:	C12H4Cl6O
SMILES:	Clc1cc(Cl)c(Oc2cc(Cl)c(Cl)cc2Cl)cc1Cl
Mol. weight [g/mol]:	376.88

Physical Properties

Property code	Value	Unit	Source
gf	40.62	kJ/mol	Joback Method
hf	-113.43	kJ/mol	Joback Method
hfus	38.95	kJ/mol	Joback Method
hvap	79.55	kJ/mol	Joback Method
log10ws	-8.36		Aqueous Solubility Prediction Method
logp	7.399		Crippen Method
mcvol	211.730	ml/mol	McGowan Method
pc	2410.00	kPa	Joback Method
tb	804.20	K	Joback Method
tc	1070.09	K	Joback Method
tf	554.71	K	Joback Method
vc	0.803	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	423.11	J/mol×K	804.20	Joback Method
cpg	453.76	J/mol×K	1025.77	Joback Method
cpg	449.28	J/mol×K	981.46	Joback Method
cpg	443.98	J/mol×K	937.14	Joback Method
cpg	437.87	J/mol×K	892.83	Joback Method
cpg	430.92	J/mol×K	848.51	Joback Method
cpg	457.46	J/mol×K	1070.09	Joback Method
dvisc	0.0001083	Paxs	804.20	Joback Method
dvisc	0.0001270	Paxs	762.62	Joback Method

dvisc	0.0001517	Paxs	721.04	Joback Method
dvisc	0.0001852	Paxs	679.46	Joback Method
dvisc	0.0002321	Paxs	637.87	Joback Method
dvisc	0.0003000	Paxs	596.29	Joback Method
dvisc	0.0004031	Paxs	554.71	Joback Method

Sources

Crippen Method:

<http://pubs.acs.org/doi/abs/10.1021/ci9903071>

Joback Method:

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

Aqueous Solubility Prediction Method:

<http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa>

McGowan Method:

<http://link.springer.com/article/10.1007/BF02311772>

Legend

cp_g:	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:	Log ₁₀ of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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