

2,2',3,4,4'-pentachlorodiphenyl ether

Inchi:	InChI=1S/C12H5Cl5O/c13-6-1-3-9(8(15)5-6)18-10-4-2-7(14)11(16)12(10)17/h1-5H
InchiKey:	RSBUDFTVQYJNHK-UHFFFAOYSA-N
Formula:	C12H5Cl5O
SMILES:	Clc1ccc(Oc2ccc(Cl)c(Cl)c2Cl)c(Cl)c1
Mol. weight [g/mol]:	342.44

Physical Properties

Property code	Value	Unit	Source
gf	62.18	kJ/mol	Joback Method
hf	-86.22	kJ/mol	Joback Method
hfus	35.15	kJ/mol	Joback Method
hvap	74.50	kJ/mol	Joback Method
log10ws	-7.44		Aqueous Solubility Prediction Method
logp	6.746		Crippen Method
mcvol	199.490	ml/mol	McGowan Method
pc	2537.93	kPa	Joback Method
tb	761.79	K	Joback Method
tc	1025.61	K	Joback Method
tf	512.27	K	Joback Method
vc	0.754	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	407.73	J/molxK	761.79	Joback Method
cpg	416.71	J/molxK	805.76	Joback Method
cpg	424.79	J/molxK	849.73	Joback Method
cpg	432.00	J/molxK	893.70	Joback Method
cpg	438.38	J/molxK	937.67	Joback Method
cpg	443.94	J/molxK	981.64	Joback Method
cpg	448.70	J/molxK	1025.61	Joback Method
dvisc	0.0005027	Paxs	512.27	Joback Method
dvisc	0.0003626	Paxs	553.86	Joback Method

dvisc	0.0002737	Paxs	595.44	Joback Method
dvisc	0.0002143	Paxs	637.03	Joback Method
dvisc	0.0001730	Paxs	678.62	Joback Method
dvisc	0.0001431	Paxs	720.20	Joback Method
dvisc	0.0001208	Paxs	761.79	Joback Method

Sources

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>

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

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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