

2,2',3,3',4,4',5,5'-octachlorodiphenyl ether

Inchi:	InChI=1S/C12H2Cl8O/c13-3-1-5(9(17)11(19)7(3)15)21-6-2-4(14)8(16)12(20)10(6)18/h1-
InchiKey:	IXZVOZCULZBCDY-UHFFFAOYSA-N
Formula:	C12H2Cl8O
SMILES:	Clc1cc(Oc2cc(Cl)c(Cl)c(Cl)c2Cl)c(Cl)c(Cl)c1Cl
Mol. weight [g/mol]:	445.77

Physical Properties

Property code	Value	Unit	Source
gf	-2.50	kJ/mol	Joback Method
hf	-167.85	kJ/mol	Joback Method
hfus	46.57	kJ/mol	Joback Method
hvap	89.64	kJ/mol	Joback Method
log10ws	-10.13		Aqueous Solubility Prediction Method
logp	8.706		Crippen Method
mcvol	236.210	ml/mol	McGowan Method
pc	2181.56	kPa	Joback Method
tb	889.02	K	Joback Method
tc	1158.50	K	Joback Method
tf	639.59	K	Joback Method
vc	0.901	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	449.36	J/molxK	889.02	Joback Method
cpg	454.97	J/molxK	933.93	Joback Method
cpg	459.75	J/molxK	978.85	Joback Method
cpg	463.70	J/molxK	1023.76	Joback Method
cpg	466.81	J/molxK	1068.67	Joback Method
cpg	469.11	J/molxK	1113.59	Joback Method
cpg	470.57	J/molxK	1158.50	Joback Method
dvisc	0.0002652	Paxs	639.59	Joback Method
dvisc	0.0002071	Paxs	681.16	Joback Method

dvisc	0.0001664	Paxs	722.73	Joback Method
dvisc	0.0001370	Paxs	764.31	Joback Method
dvisc	0.0001150	Paxs	805.88	Joback Method
dvisc	0.0000982	Paxs	847.45	Joback Method
dvisc	0.0000851	Paxs	889.02	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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