Isobenzan

Other names:	4,7-Methanoisobenzofuran, 1,3,4,5,6,7,8,8-octachloro-1,3,3a,4,7,7a-hexahydro- CP 14,957 ENT 25,545-X Shell WL 1650 SD 4402 Telodrin WL 1650 948 1,3,4,5,6,7,8,8-Octachloro-1,3,3a,4,7,7a-hexahydro-4,7-methanoisobenzofuran ENT 25,545 Octachloro-hexahydro-methanoisobenzofuran 1,3,4,5,6,8,8-Octachloro-1,3,3a,4,7,7a-hexahydro-4,7-methanoisobenzofuran 1,3,4,5,6,7,8,8-Octachloro-2-oxa-3a,4,7,7a-tetrahydro-4,7-methanoindene 1,3,4,5,6,7,10,10-Octachloro-4,7-endo-methylene-4,7,8,9-tetrahydrophthalan OMS 206 Omtan R 6700 Shell 4402 4,7-Methanoisobenzofuran, 1,3,4,5,6,7,8,8-octachloro-3a,4,7,7a-tetrahydro-
Inchi:	InChI=1S/C9H4Cl8O/c10-3-4(11)8(15)2-1(5(12)18-6(2)13)7(3,14)9(8,16)17/h1-2,5-6H
InchiKey:	LRWHHSXTGZSMSN-UHFFFAOYSA-N
Formula:	C9H4Cl8O
SMILES:	ClC1=C(Cl)C2(Cl)C3C(Cl)OC(Cl)C3C1(Cl)C2(Cl)Cl
Mol. weight [g/mol]:	411.75
CAS:	297-78-9

Physical Properties

Property code	Value	Unit	Source
gf	-23.12	kJ/mol	Joback Method
hf	-275.57	kJ/mol	Joback Method
hfus	38.76	kJ/mol	Joback Method
hvap	72.06	kJ/mol	Joback Method
log10ws	-5.99		Crippen Method
logp	5.224		Crippen Method
mcvol	204.580	ml/mol	McGowan Method
pc	2595.13	kPa	Joback Method
tb	747.36	K	Joback Method

tc	1027.18	K	Joback Method
tf	395.40 ± 0.20	K	NIST Webbook
vc	0.791	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	437.42	J/mol×K	747.36	Joback Method
cpg	448.19	J/mol×K	794.00	Joback Method
cpg	460.30	J/mol×K	840.63	Joback Method
cpg	474.48	J/mol×K	887.27	Joback Method
cpg	491.43	J/mol×K	933.91	Joback Method
cpg	511.85	J/mol×K	980.54	Joback Method
cpg	536.46	J/mol×K	1027.18	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C297789&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method: https://en.wikipedia.org/wiki/Joback_method
McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Legend

cpg: Ideal gas heat capacity
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