p,p'-DDT

Other names:

1,1'-(2,2,2,-Trichloroethylidene)bis[4-chlorobenzene]
1,1,1-Trichloor-2,2-bis(4-chloor fenyl)-ethaan
1,1,1-Trichlor-2,2-bis(4-chlor-phenyl)-aethan
1,1,1-Trichloro-2,2-bis(4,4'-dichlorodiphenyl)ethane
1,1,1-Trichloro-2,2-bis(4-chlorophenyl)ethane (pp'DDT)
1,1,1-Trichloro-2,2-bis(p-chlorophenyl)ethane
1,1,1-Trichloro-2,2-di(4-chlorophenyl)ethane
1,1,1-Tricloro-2,2-bis(4-cloro-fenil)-etano
1,1,1-trichloro-2-2-bis(4-chlorophenyl)ethane
1,1-Bis(4-chlorophenyl)-2,2,2-trichloroethane
1,1-bis(p-Chlorophenyl)-2,2,2-trichloroethane
1-chloro-4-[2,2,2-trichloro-1-(4-chlorophenyl)ethyl]benzene
2,2,2-Trichloro-1,1-bis(4-chlorophenyl)ethane
2,2-Bis(p-chlorophenyl)-1,1,1-trichloroethane
4,4'-DDT
4,4'-Dichlorodiphenyltrichloroethane
Aavero-extra
Agritan
Anofex
Arkotine
Azotox
Azotox M-33
Benzene, 1,1'-(2,2,2-trichloroethylidene)bis[4-chloro-
Benzochloryl
Bosan supra
Bovidermol
Chlorophenothan
Chlorophenothane
Chlorophenotoxum
Chlorphenothan
Chlorphenotoxum
Citox
Clofenotan
Clofenotane
DDT
DDT(p,p')
Dedelo
Deoval
Detox
Detoxan

Dibovan
Dibovin
Dicophane
Dicophaner
Didigam
Didimac
Dodat
Dykol
ENT 1,506
ENT-1506
Estonate
Ethane, 1,1,1-Trichloro-2,2-bis(p-chlorophenyl)-
Ethane, 1,1,1-trichloro-2,2-bis(4-chlorophenyl)-
Genitox
Gesafid
Gesapon
Gesarex
Gesarol
Geusapon
Guesapon
Guesarol
Gyron
Havero-extra
Hildit
Ivoran
Ixodex
Kopsol
Micro DDT 75
Mutoxan
Mutoxin
NCI-C00464
Neocid
Neocidol
Neocidol, Solid
OMS 16
PEB1
Parachlorocidum
Pentachlorin
Pentech
Penticide
Penticidum
R50
RCRA Waste number U061

	Rukseam
	Santobane
	Tafidex
	Trichlorobis(4'-Chlorophenyl)ethane
	Trichlorobis(4-chlorophenyl)ethane
	Zeidane
	Zerdane
	p,p'-Dichlorodiphenyltrichloroethane
	p,p'-Dichlorodiphenyltrichloromethylmethane
	p,p-DDT
	pPzeidan
	«alpha»,«alpha»-Bis(p-chlorophenyl)-«beta»,«beta»,«beta»-trichlorethane
	Â«alphaÂ»,Â«alphaÂ»-Bis(p-chlorophenyl)-Â«betaÂ»,Â«betaÂ»,Â«betaÂ»-trichlorethane
Inchi:	InChI=1S/C14H9Cl5/c15-11-5-1-9(2-6-11)13(14(17,18)19)10-3-7-12(16)8-4-10/h1-8,13H
InchiKey:	YVGGHNCTFXOJCH-UHFFFAOYSA-N
Formula:	C14H9Cl5
SMILES:	Clc1ccc(C(c2ccc(Cl)cc2)C(Cl)(Cl)Cl)cc1
Mol. weight [g/mol]:	354.49
CAS:	50-29-3

Physical Properties

Property code	Value	Unit	Source
gf	213.31	kJ/mol	Joback Method
hf	25.10	kJ/mol	Joback Method
hfus	29.37	kJ/mol	Joback Method
hvap	72.88	kJ/mol	Joback Method
log10ws	-7.40		Aqueous Solubility Prediction Method
log10ws	-7.15		Estimated Solubility Method
logp	6.495		Crippen Method
mcvol	221.800	ml/mol	McGowan Method
pc	2293.71	kPa	Joback Method
rinpol	2300.00		NIST Webbook
rinpol	2300.00		NIST Webbook
rinpol	2299.00		NIST Webbook
rinpol	2270.00		NIST Webbook
rinpol	2325.20		NIST Webbook
rinpol	2330.00		NIST Webbook
rinpol	2290.00		NIST Webbook

rinpol	2289.00		NIST Webbook
rinpol	2301.00		NIST Webbook
rinpol	2284.00		NIST Webbook
rinpol	2284.00		NIST Webbook
rinpol	2330.00		NIST Webbook
rinpol	2290.00		NIST Webbook
rinpol	2325.20		NIST Webbook
rinpol	2263.00		NIST Webbook
rinpol	2270.00		NIST Webbook
rinpol	2277.00		NIST Webbook
rinpol	2264.00		NIST Webbook
rinpol	2270.00		NIST Webbook
rinpol	2277.00		NIST Webbook
rinpol	2264.00		NIST Webbook
rinpol	2300.00		NIST Webbook
rinpol	2270.00		NIST Webbook
rinpol	2289.00		NIST Webbook
ripol	3106.00		NIST Webbook
ripol	3103.00		NIST Webbook
ripol	3103.00		NIST Webbook
ripol	3106.00		NIST Webbook
ripol	3106.00		NIST Webbook
tb	766.52	K	Joback Method
tc	1041.34	K	Joback Method
tf	381.95	K	Aqueous Solubility Prediction Method
tf	383.17 ± 0.20	K	NIST Webbook
tf	383.00 ± 0.20	K	NIST Webbook
tf	382.25 ± 1.00	K	NIST Webbook
vc	0.832	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	495.29	J/mol×K	766.52	Joback Method
cpg	506.48	J/mol×K	812.32	Joback Method
cpg	516.50	J/mol×K	858.13	Joback Method
cpg	525.51	J/mol×K	903.93	Joback Method
cpg	533.67	J/mol×K	949.73	Joback Method
cpg	541.13	J/mol×K	995.53	Joback Method
cpg	548.06	J/mol×K	1041.34	Joback Method

dvisc	0.0001157	Pa×s	715.84	Joback Method
dvisc	0.0001547	Pa×s	665.16	Joback Method
dvisc	0.0002169	Pa×s	614.48	Joback Method
dvisc	0.0003233	Pa×s	563.80	Joback Method
dvisc	0.0005214	Pa×s	513.12	Joback Method
dvisc	0.0000899	Pa×s	766.52	Joback Method
dvisc	0.0009338	Pa×s	462.44	Joback Method
hfust	26.28	kJ/mol	382.10	NIST Webbook
hsubt	118.00	kJ/mol	356.00	NIST Webbook
hsubt	115.00	kJ/mol	343.00	NIST Webbook
hsubt	120.20 ± 1.00	kJ/mol	293.00	NIST Webbook
hsubt	84.00	kJ/mol	338.00	NIST Webbook
hsubt	117.80	kJ/mol	303.00	NIST Webbook
hsubt	110.00	kJ/mol	323.00	NIST Webbook
hsubt	117.50	kJ/mol	343.00	NIST Webbook
hvapt	106.10 ± 1.30	kJ/mol	398.00	NIST Webbook
hvapt	93.20	kJ/mol	398.00	NIST Webbook
hvapt	338.00	kJ/mol	338.00	NIST Webbook

Sources

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Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Joback Method: https://en.wikipedia.org/wiki/Joback_method
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
McGowan Method: http://link.springer.com/article/10.1007/BF02311772

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
hfust: Enthalpy of fusion at a given temperature
hsubt: Enthalpy of sublimation at a given temperature
hvap: Enthalpy of vaporization at standard conditions
hvapt: Enthalpy of vaporization at a given temperature

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume