Methoxychlor

Other names:

1,1'-(2,2,2-Trichloroethylidene)bis(4-methoxybenzene)
1,1,1-Trichlor-2,2-bis(4-methoxy-phenyl)-aethan
1,1,1-Trichloro-2,2-bis(4-methoxyphenyl)ethane
1,1,1-Trichloro-2,2-bis(p-anisyl)ethane
1,1,1-Trichloro-2,2-bis(p-methoxyphenyl)ethane
1,1,1-Trichloro-2,2-di(4-methoxyphenyl)ethane
1,1-Bis(p-methoxyphenyl)-2,2,2-trichloroethane
1-methoxy-4-[2,2,2-trichloro-1-(4-methoxyphenyl)ethyl]benzene
2,2,2-Trichloro-1,1-bis(4-methoxyphenyl)ethane
2,2-Bis (p-methoxyphenol)-1,1,1-trichloroethane
2,2-Bis(p-anisyl)-1,1,1-trichloroethane
2,2-Bis(p-methoxyphenyl)-1,1,1-trichloroethane
2,2-Di(p-anisyl)-1,1,1-trichloroethane
2,2-Di(p-methoxyphenyl)-1,1,1-trichloroethane
4,4-(2,2,2-Trichloroethylidene)dianisole
Benzene, 1,1'-(2,2,2-trichloroethylidene)bis*4-methoxy-
Benzene, 1,1'-(2,2,2-trichloroethylidene)bis[4-methoxy-
Chemform
DMDT
Di(p-methoxyphenyl)trichloromethyl methane
Dianisyltrichlorethane
Dimethoxy-DDT
Dimethoxy-dt
Double-M ec
ENT 1,716
Ethane, 1,1,1-trichloro-2,2-bis(p-methoxyphenyl)-
Ethane, 2,2-bis(p-anisyl)-1,1,1-trichloro-
Flo pro mcseed protectant
Higalmetox
Maralate
Marlate
MeOCl
Mesox K
Methoxcide
Methoxy-DDT
Methoxychlor 2 EC
Methoxychlore
Metoksychlor
Metox
Mezox K

Moxie
NCI-C00497
OMS 466
RCRA Waste number U247
p,p'-(Dimethoxydiphenyl)trichloroethane
p,p'-DMDT
p,p'-Dwumetoksydwufenylotrojchloroetan
p,p'-Methoxychlor
pMethoxychlor

Inchi: InChI=1S/C16H15Cl3O2/c1-20-13-7-3-11(4-8-13)15(16(17,18)19)12-5-9-14(21-2)10-6-12

InchiKey: IAKOZHOLGAGEJT-UHFFFAOYSA-N

Formula: C16H15Cl3O2

SMILES: COc1ccc(C(c2ccc(OC)cc2)C(Cl)(Cl)Cl)cc1

Mol. weight [g/mol]: 345.65

CAS: 72-43-5

Physical Properties

Property code	Value	Unit	Source
gf	44.01	kJ/mol	Joback Method
hf	-249.14	kJ/mol	Joback Method
hfus	28.53	kJ/mol	Joback Method
hvap	73.38	kJ/mol	Joback Method
log10ws	-6.89		Estimated Solubility Method
log10ws	-6.59		Aqueous Solubility Prediction Method
logp	5.206		Crippen Method
mcvol	237.240	ml/mol	McGowan Method
pc	1992.98	kPa	Joback Method
rinpol	2413.00		NIST Webbook
rinpol	2420.00		NIST Webbook
rinpol	2491.00		NIST Webbook
rinpol	2395.00		NIST Webbook
rinpol	2439.30		NIST Webbook
rinpol	2410.00		NIST Webbook
rinpol	2418.00		NIST Webbook
rinpol	2401.00		NIST Webbook
rinpol	2417.00		NIST Webbook
rinpol	2420.00		NIST Webbook
rinpol	2420.00		NIST Webbook

rinpol	2417.00		NIST Webbook
tb	782.26	K	Joback Method
tc	1032.53	K	Joback Method
tf	362.70 ± 0.20	K	NIST Webbook
tf	361.56 ± 0.20	K	NIST Webbook
vc	0.881	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	606.37	J/mol×K	782.26	Joback Method
cpg	620.25	J/mol×K	823.97	Joback Method
cpg	632.84	J/mol×K	865.68	Joback Method
cpg	644.21	J/mol×K	907.40	Joback Method
cpg	654.43	J/mol×K	949.11	Joback Method
cpg	663.59	J/mol×K	990.82	Joback Method
cpg	671.75	J/mol×K	1032.53	Joback Method
dvisc	0.0005631	Pa×s	469.60	Joback Method
dvisc	0.0003092	Pa×s	521.71	Joback Method
dvisc	0.0001893	Pa×s	573.82	Joback Method
dvisc	0.0001258	Pa×s	625.93	Joback Method
dvisc	0.0000890	Pa×s	678.04	Joback Method
dvisc	0.0000662	Pa×s	730.15	Joback Method
dvisc	0.0000512	Pa×s	782.26	Joback Method
hfust	27.48	kJ/mol	360.60	NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C72435&Units=SI

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

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
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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume