2,2-Bis(p-methoxyphenyl)-1,1-dichloroethylene

Other names:	Methoxychlor olefin
	Benzene, 1,1'-(dichloroethenylidene)bis[4-methoxy-
	Ethylene, 1,1-dichloro-2,2-bis(p-methoxyphenyl)-
	p,p'-Methoxychlor olefin
	DMDE
	1,1-Bis(p-methoxyphenyl)-2,2-dichloroethylene
	1,1-Dichloro-2,2-bis(p-methoxyphenyl)ethylene
	1,1-Dichloro-2,2-bis(4-methoxyphenyl) ethene
	2,2-Dichloro-1,1-bis(4-methoxyphenyl)ethylene
	p,p-Methoxychlor olefin
	1,1-Dichloro-2,2-bis(4-methoxyphenyl)ethylene
	NSC 97452
	Methoxychlor olefin (DDE-analog)
	Methoxychlor, dehydrochloro
Inchi:	InChI=1S/C16H14Cl2O2/c1-19-13-7-3-11(4-8-13)15(16(17)18)12-5-9-14(20-2)10-6-12/h3
InchiKey:	YCRYSVKEWAWTGI-UHFFFAOYSA-N
Formula:	C16H14Cl2O2
SMILES:	COc1ccc(C(=C(Cl)Cl)c2ccc(OC)cc2)cc1
Mol. weight [g/mol]:	309.19
CAS:	2132-70-9

Physical Properties

Property code	Value	Unit	Source
gf	118.66	kJ/mol	Joback Method
hf	-121.73	kJ/mol	Joback Method
hfus	32.85	kJ/mol	Joback Method
hvap	70.79	kJ/mol	Joback Method
log10ws	-5.55		Crippen Method
logp	4.898		Crippen Method
mcvol	220.700	ml/mol	McGowan Method
pc	2127.56	kPa	Joback Method
tb	752.42	K	Joback Method
tc	999.84	K	Joback Method
tf	419.26	K	Joback Method
vc	0.832	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	554.05	J/mol×K	752.42	Joback Method
cpg	568.49	J/mol×K	793.66	Joback Method
cpg	581.74	J/mol×K	834.89	Joback Method
cpg	593.86	J/mol×K	876.13	Joback Method
cpg	604.91	J/mol×K	917.36	Joback Method
cpg	614.95	J/mol×K	958.60	Joback Method
cpg	624.04	J/mol×K	999.84	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C2132709&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