p,p'-Methoxychlor olefin

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

Physical Properties

Property code	Value	Unit	Source
hf	-80.20	kJ/mol	Cheméo Relay (1.0)
hfus	32.85	kJ/mol	Joback Method
hvap	90.41	kJ/mol	Cheméo Relay (1.0)
ie	7.46	eV	Cheméo Relay (1.0)
log10ws	-5.89		Cheméo Relay (1.0)
logp	4.898		Crippen Method
mcvol	220.700	ml/mol	McGowan Method
pc	2127.56	kPa	Joback Method
tb	645.92	K	Cheméo Relay (1.0)
tc	890.37	K	Cheméo Relay (1.0)
tf	377.88	K	Cheméo Relay (1.0)

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

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C2132709&Units=SI

Legend

cpg:	Ideal gas heat capacity
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
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