o,p'-Methoxychlor

Other names: Benzene, 1-methoxy-2-[2,2,2-trichloro-1-(4-methoxyphenyl)ethyl]-
Ethane, 1,1,1-trichloro-2-(o-methoxyphenyl)-2-(p-methoxyphenyl)-
o,p-Methoxychlor
1-Methoxy-2-(2,2,2-tricloro-1-(4-methoxyphenyl)ethyl)benzene
Inchi: InChI=1S/C16H15Cl3O2/c1-20-12-9-7-11(8-10-12)15(16(17,18)19)13-5-3-4-6-14(13)21-2
InchiKey: KNLLPAOBVIKLDE-UHFFFAOYSA-N
Formula: C16H15Cl3O2
SMILES: COc1ccc(C(c2ccccc2OC)C(Cl)(Cl)Cl)cc1
Mol. weight [g/mol]: 345.65
CAS: 30667-99-3

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	-5.76		Crippen Method
logp	5.206		Crippen Method
mcvol	237.240	ml/mol	McGowan Method
pc	1992.98	kPa	Joback Method
tb	782.26	K	Joback Method
tc	1032.53	K	Joback Method
tf	349.72 ± 0.20	K	NIST Webbook
vc	0.881	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	671.75	J/mol×K	1032.53	Joback Method
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
dvisc	0.0000512	Pa×s	782.26	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
hfust	22.45	kJ/mol	347.60	NIST Webbook

Sources

Joback Method: https://en.wikipedia.org/wiki/Joback_method
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C30667993&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

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
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume

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