Benzene, 1-methoxy-2-[2,2,2-trichloro-1-(4-methoxyphenyl)e

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

Physical Properties

Property code	Value	Unit	Source
hfus	28.53	kJ/mol	Joback Method
log10ws	-6.20		Cheméo Relay (1.0)
logp	5.206		Crippen Method
mcvol	237.240	ml/mol	McGowan Method
tf	349.72 ± 0.20	K	NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	663.59	J/mol×K	990.82	Joback Method
cpg	671.75	J/mol×K	1032.53	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	606.37	J/mol×K	782.26	Joback Method
dvisc	0.0001893	Pa×s	573.82	Joback Method
dvisc	0.0003092	Pa×s	521.71	Joback Method
dvisc	0.0005631	Pa×s	469.60	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	22.45	kJ/mol	347.60	NIST Webbook

Sources

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=C30667993&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
hfus:	Enthalpy of fusion at standard conditions
hfust:	Enthalpy of fusion at a given temperature
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tf:	Normal melting (fusion) point