Benzene, 1,2,3,4-tetrachloro-5-methoxy-

Other names:	1,2,3,4-tetrachloro-5-methoxybenzene
	2,3,4,5-Tetrachloroanisole
	2,4,3,5-tetrachloroanisole
	Anisole, 2,3,4,5-tetrachloro-
Inchi:	InChI=1S/C7H4Cl4O/c1-12-4-2-3(8)5(9)7(11)6(4)10/h2H,1H3
InchiKey:	FUUHMSUPRUNWRQ-UHFFFAOYSA-N
Formula:	C7H4Cl4O
SMILES:	COc1cc(Cl)c(Cl)c(Cl)c1Cl
Mol. weight [g/mol]:	245.92
CAS:	938-86-3

Physical Properties

Property code	Value	Unit	Source
gf	-70.77	kJ/mol	Joback Method
hf	-192.34	kJ/mol	Joback Method
hfus	24.35	kJ/mol	Joback Method
hvap	56.05	kJ/mol	Joback Method
log10ws	-5.26		Aqueous Solubility Prediction Method
logp	4.309		Crippen Method
mcvol	140.560	ml/mol	McGowan Method
pc	3142.03	kPa	Joback Method
rinpol	1644.00		NIST Webbook
rinpol	1629.00		NIST Webbook
rinpol	1660.00		NIST Webbook
rinpol	1649.00		NIST Webbook
rinpol	1633.00		NIST Webbook
rinpol	1660.00		NIST Webbook
rinpol	1618.00		NIST Webbook
rinpol	1620.00		NIST Webbook
ripol	2336.00		NIST Webbook
ripol	2362.00		NIST Webbook
ripol	2369.00		NIST Webbook
ripol	2367.00		NIST Webbook
ripol	2340.00		NIST Webbook
ripol	2319.00		NIST Webbook
tb	578.30	K	Joback Method

tc	816.84	K	Joback Method
tf	387.06	K	Joback Method
vc	0.533	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	245.24	J/mol×K	578.30	Joback Method
cpg	252.60	J/mol×K	618.06	Joback Method
cpg	259.55	J/mol×K	657.81	Joback Method
cpg	266.09	J/mol×K	697.57	Joback Method
cpg	272.20	J/mol×K	737.33	Joback Method
cpg	277.88	J/mol×K	777.08	Joback Method
cpg	283.12	J/mol×K	816.84	Joback Method
dvisc	0.0008652	Pa×s	387.06	Joback Method
dvisc	0.0006311	Pa×s	418.93	Joback Method
dvisc	0.0004813	Pa×s	450.81	Joback Method
dvisc	0.0003804	Pa×s	482.68	Joback Method
dvisc	0.0003096	Pa×s	514.55	Joback Method
dvisc	0.0002581	Pa×s	546.43	Joback Method
dvisc	0.0002195	Pa×s	578.30	Joback Method

Sources

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
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C938863&Units=SI

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