Benzene, 1,2,3,4-tetrachloro-5,6-dimethoxy-

Other names: 1,2,3,4-Tetrachloro-5,6-dimethoxybenzene
Tetrachloroveratrole
Inchi: InChI=1S/C8H6Cl4O2/c1-13-7-5(11)3(9)4(10)6(12)8(7)14-2/h1-2H3
InchiKey: NCYHCGGUQGDEQW-UHFFFAOYSA-N
Formula: C8H6Cl4O2
SMILES: COc1c(Cl)c(Cl)c(Cl)c(Cl)c1OC
Mol. weight [g/mol]: 275.94
CAS: 944-61-6

Physical Properties

Property code	Value	Unit	Source
gf	-176.98	kJ/mol	Joback Method
hf	-356.67	kJ/mol	Joback Method
hfus	27.74	kJ/mol	Joback Method
hvap	61.35	kJ/mol	Joback Method
log10ws	-5.24		Aqueous Solubility Prediction Method
logp	4.317		Crippen Method
mcvol	160.520	ml/mol	McGowan Method
pc	2735.42	kPa	Joback Method
rinpol	1677.00		NIST Webbook
rinpol	1690.00		NIST Webbook
rinpol	1705.00		NIST Webbook
rinpol	1724.00		NIST Webbook
rinpol	1677.00		NIST Webbook
rinpol	1726.00		NIST Webbook
rinpol	1726.00		NIST Webbook
ripol	2359.00		NIST Webbook
ripol	2342.00		NIST Webbook
ripol	2301.00		NIST Webbook
ripol	2301.00		NIST Webbook
ripol	2331.00		NIST Webbook
tb	628.58	K	Joback Method
tc	859.87	K	Joback Method
tf	433.08	K	Joback Method
vc	0.608	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	307.99	J/mol×K	628.58	Joback Method
cpg	345.68	J/mol×K	821.32	Joback Method
cpg	339.12	J/mol×K	782.77	Joback Method
cpg	332.04	J/mol×K	744.23	Joback Method
cpg	324.47	J/mol×K	705.68	Joback Method
cpg	316.44	J/mol×K	667.13	Joback Method
cpg	351.69	J/mol×K	859.87	Joback Method
dvisc	0.0001570	Pa×s	628.58	Joback Method
dvisc	0.0001831	Pa×s	596.00	Joback Method
dvisc	0.0002174	Pa×s	563.41	Joback Method
dvisc	0.0002637	Pa×s	530.83	Joback Method
dvisc	0.0003279	Pa×s	498.25	Joback Method
dvisc	0.0004205	Pa×s	465.66	Joback Method
dvisc	0.0005597	Pa×s	433.08	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C944616&Units=SI

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

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