1,3-Cyclopentadiene, 1,2,3,4-tetrachloro-5,5-dimethoxy-

Other names:	5,5-Dimethoxy-1,2,3,4-tetrachlorocyclopentadiene
	2,4-Cyclopentadien-1-one, 2,3,4,5-tetrachloro-, dimethyl acetal
	1,2,3,4-Tetrachloro-5,5-dimethoxycyclopentadiene
	5,5-Dimethoxytetrachlorocyclopentadiene
	Tetrachlorocyclopentadienone dimethyl acetal
	2,3,4,5-Tetrachlorocyclopentadienone dimethyl acetal
	2,3,4,5-Tetrachloro-1,1-dimethoxycyclopentadiene
	Tetrachlorocyclopentadienone dimethyl ketal
	1,1-Dimethoxy-2,3,4,5-tetrachlorocyclopentadiene
	Cyclopentadienone, tetrachloro-, dimethyl acetal
	1, 2, 3, 4-Tetrachloro-5, 5-dimethoxy-1,3-cyclopentadiene
	1,2,3,4-tetrachloro-5,5-dimethoxycyclopenta-1,3-diene
Inchi:	InChI=1S/C7H6Cl4O2/c1-12-7(13-2)5(10)3(8)4(9)6(7)11/h1-2H3
InchiKey:	UHSMEJQTFMHABA-UHFFFAOYSA-N
Formula:	C7H6Cl4O2
SMILES:	COC1(OC)C(Cl)=C(Cl)C(Cl)=C1Cl
Mol. weight [g/mol]:	263.93
CAS:	2207-27-4

Physical Properties

Property code	Value	Unit	Source
gf	-197.20	kJ/mol	Joback Method
hf	-369.81	kJ/mol	Joback Method
hfus	21.58	kJ/mol	Joback Method
hvap	55.87	kJ/mol	Joback Method
log10ws	-3.73		Crippen Method
logp	3.367		Crippen Method
mcvol	150.730	ml/mol	McGowan Method
pc	2969.80	kPa	Joback Method
tb	587.88	K	Joback Method
tc	820.92	K	Joback Method
tf	419.19	K	Joback Method
vc	0.571	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	287.77	J/mol×K	587.88	Joback Method
cpg	295.77	J/mol×K	626.72	Joback Method
cpg	303.41	J/mol×K	665.56	Joback Method
cpg	310.76	J/mol×K	704.40	Joback Method
cpg	317.91	J/mol×K	743.24	Joback Method
cpg	324.95	J/mol×K	782.08	Joback Method
cpg	331.96	J/mol×K	820.92	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	382.20	K	1.50	NIST Webbook
tbrp	358.00 ± 6.00	K	0.08	NIST Webbook

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
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=C2207274&Units=SI

Legend

cpg: Ideal gas heat capacity
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
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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