Perchlorocyclobutenone

Other names:	2-Cyclobuten-1-one, 2,3,4,4-tetrachloro-
	Perchloro-2-cyclobuten-1-one
	Perchloro-2-cyclobutene-1-one
	Perchlorocyclobut-2-enone
	Tetrachlorocyclobutenone
	tetrachlorocyclobut-2-enone
Inchi:	InChI=1S/C4Cl4O/c5-1-2(6)4(7,8)3(1)9
InchiKey:	NWDONRNKYCKRNT-UHFFFAOYSA-N
Formula:	C4Cl4O
SMILES:	O=C1C(Cl)=C(Cl)C1(Cl)Cl
Mol. weight [g/mol]:	205.85
CAS:	3200-96-2

Physical Properties

Property code	Value	Unit	Source
gf	-133.65	kJ/mol	Joback Method
hf	-209.83	kJ/mol	Joback Method
hfus	12.60	kJ/mol	Joback Method
hvap	46.84	kJ/mol	Joback Method
log10ws	-2.74		Crippen Method
logp	2.432		Crippen Method
mcvol	102.590	ml/mol	McGowan Method
pc	4391.59	kPa	Joback Method
tb	528.83	K	Joback Method
tc	785.85	K	Joback Method
tf	386.86	K	Joback Method
vc	0.396	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	159.47	J/mol×K	528.83	Joback Method
cpg	164.01	J/mol×K	571.67	Joback Method
cpg	168.16	J/mol×K	614.50	Joback Method

cpg	172.03	J/mol×K	657.34	Joback Method
cpg	175.78	J/mol×K	700.18	Joback Method
cpg	179.52	J/mol×K	743.02	Joback Method
cpg	183.39	J/mol×K	785.85	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C3200962&Units=SI
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

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