Endolactone

Other names:	4,7-Methanoisobenzofuran-1(3H)-one, 4,5,6,7,8,8-hexachloro-3a,4,7,7a-tetrahydro-, «gamma»-lactone 5-Norbornene-2-carboxylic acid, 1,4,5,6,7,7-hexachloro-3-(hydroxymethyl)-, Endosulfan lactone
Inchi:	InChI=1S/C9H4Cl6O2/c10-4-5(11)8(13)3-2(1-17-6(3)16)7(4,12)9(8,14)15/h2-3H,1H2
InchiKey:	GIUKJJMBQBRFTN-UHFFFAOYSA-N
Formula:	C9H4Cl6O2
SMILES:	O=C1OCC2C1C1(Cl)C(Cl)=C(Cl)C2(Cl)C1(Cl)Cl
Mol. weight [g/mol]:	356.85
CAS:	3868-61-9

Physical Properties

Property code	Value	Unit	Source
gf	-106.43	kJ/mol	Joback Method
hf	-341.11	kJ/mol	Joback Method
hfus	27.73	kJ/mol	Joback Method
hvap	68.15	kJ/mol	Joback Method
log10ws	-4.25		Crippen Method
logp	3.621		Crippen Method
mcvol	181.670	ml/mol	McGowan Method
pc	3127.99	kPa	Joback Method
tb	749.66	K	Joback Method
tc	1036.37	K	Joback Method
tf	604.82	K	Joback Method
vc	0.703	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	406.43	J/mol×K	749.66	Joback Method
cpg	417.83	J/mol×K	797.44	Joback Method
cpg	430.68	J/mol×K	845.23	Joback Method
cpg	445.70	J/mol×K	893.01	Joback Method
cpg	463.60	J/mol×K	940.80	Joback Method
cpg	485.09	J/mol×K	988.58	Joback Method

cpg	510.89	J/mol×K	1036.37	Joback Method

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=C3868619&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
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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