Chlorendic anhydride

Other names:	4,7-Methanoisobenzofuran-1,3-dione, 4,5,6,7,8,8-hexachloro-3a,4,7,7a-tetrahydro- 5-Norbornene-2,3-dicarboxylic anhydride, 1,4,5,6,7,7-hexachloro- Chloran 542 Hexachloro-5-norbornene-2,3-dicarboxylic anhydride Hexachloroendomethylene tetrahydrophthalic anhydride HET Anhydride 1,4,5,6,7,7-Hexachloro-5-norbornene-2,3-dicarboxylic anhydride 1,4,5,6,7,7-Hexachlorobicyclo [2.2.1]hept-5-ene-2,3-dicarboxylic anhydride 1,4,5,6,7,7-Hexachlorobicyclo[2.2.1]-5-heptene-2,3-dicarboxylic acid anhydride Bicyclo[2.2.1]hept-5-ene-2,3-dicarboxylic anhydride, 1,4,5,6,7,7-hexachloro- NSC 22229 1,4,5,6,7,7-hexachloro-8,9,10-trinorborn-5-ene-2,3-dicarboxylic anhydride
Inchi:	InChI=1S/C9H2Cl6O3/c10-3-4(11)8(13)2-1(5(16)18-6(2)17)7(3,12)9(8,14)15/h1-2H
InchiKey:	FLBJFXNAEMSXGL-UHFFFAOYSA-N
Formula:	C9H2Cl6O3
SMILES:	O=C1OC(=O)C2C1C1(Cl)C(Cl)=C(Cl)C2(Cl)C1(Cl)Cl
Mol. weight [g/mol]:	370.83
CAS:	115-27-5

Physical Properties

Property code	Value	Unit	Source
gf	-229.02	kJ/mol	Joback Method
hf	-478.81	kJ/mol	Joback Method
hfus	27.24	kJ/mol	Joback Method
hvap	72.40	kJ/mol	Joback Method
log10ws	-4.02		Crippen Method
logp	3.148		Crippen Method
mcvol	183.240	ml/mol	McGowan Method
pc	3254.14	kPa	Joback Method
tb	817.48	K	Joback Method
tc	1113.33	K	Joback Method
tf	673.04	K	Joback Method
vc	0.710	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	423.17	J/mol×K	817.48	Joback Method
cpg	437.43	J/mol×K	866.79	Joback Method
cpg	454.09	J/mol×K	916.10	Joback Method
cpg	473.86	J/mol×K	965.41	Joback Method
cpg	497.45	J/mol×K	1014.71	Joback Method
cpg	525.54	J/mol×K	1064.02	Joback Method
cpg	558.85	J/mol×K	1113.33	Joback Method

Sources

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=C115275&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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