2,2,4,4,6-Pentachloro-5-cyclohexene-1,3-dione

Inchi: InChI=1S/C6HCl5O2/c7-2-1-5(8,9)4(13)6(10,11)3(2)12/h1H
InchiKey: NTFAWJMNLRUDJB-UHFFFAOYSA-N
Formula: C6HCl5O2
SMILES: O=C1C(Cl)=CC(Cl)(Cl)C(=O)C1(Cl)Cl
Mol. weight [g/mol]: 282.34
CAS: 15679-05-7

Physical Properties

Property code	Value	Unit	Source
gf	-279.10	kJ/mol	Joback Method
hf	-410.50	kJ/mol	Joback Method
hfus	12.44	kJ/mol	Joback Method
hvap	58.14	kJ/mol	Joback Method
log10ws	-3.12		Crippen Method
logp	2.609		Crippen Method
mcvol	144.580	ml/mol	McGowan Method
pc	3782.33	kPa	Joback Method
tb	678.97	K	Joback Method
tc	970.46	K	Joback Method
tf	507.64	K	Joback Method
vc	0.544	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	272.98	J/mol×K	678.97	Joback Method
cpg	281.60	J/mol×K	727.55	Joback Method
cpg	290.33	J/mol×K	776.13	Joback Method
cpg	299.47	J/mol×K	824.72	Joback Method
cpg	309.33	J/mol×K	873.30	Joback Method
cpg	320.19	J/mol×K	921.88	Joback Method
cpg	332.37	J/mol×K	970.46	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=C15679057&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