1,3-Isobenzofurandione, 5,6-dichloro-

Other names: 4,5-dichlorophthalic anhydride
Inchi: InChI=1S/C8H2Cl2O3/c9-5-1-3-4(2-6(5)10)8(12)13-7(3)11/h1-2H
InchiKey: ULSOWUBMELTORB-UHFFFAOYSA-N
Formula: C8H2Cl2O3
SMILES: O=C1OC(=O)c2cc(Cl)c(Cl)cc21
Mol. weight [g/mol]: 217.01
CAS: 942-06-3

Physical Properties

Property code	Value	Unit	Source
gf	-186.70	kJ/mol	Joback Method
hf	-352.07	kJ/mol	Joback Method
hfus	21.81	kJ/mol	Joback Method
hvap	59.66	kJ/mol	Joback Method
log10ws	-3.30		Crippen Method
logp	2.304		Crippen Method
mcvol	122.450	ml/mol	McGowan Method
pc	4162.33	kPa	Joback Method
tb	586.20	K	NIST Webbook
tc	943.03	K	Joback Method
tf	488.93	K	Joback Method
vc	0.467	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	263.24	J/mol×K	672.92	Joback Method
cpg	272.28	J/mol×K	717.94	Joback Method
cpg	280.63	J/mol×K	762.96	Joback Method
cpg	288.24	J/mol×K	807.97	Joback Method
cpg	295.10	J/mol×K	852.99	Joback Method
cpg	301.16	J/mol×K	898.01	Joback Method
cpg	306.40	J/mol×K	943.03	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C942063&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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