1,3-Isobenzofurandione, 4,5,6,7-tetrachloro-

Other names:	Phthalic anhydride, tetrachloro- Niagathal Tetrachlorophthalic anhydride 1,3-Dioxo-4,5,6,7-tetrachloroisobenzofuran NCI-C61585 3,4,5,6-Tetrachlorophthalic anhydride Tetrachlorophthalic acid anhydride 4,5,6,7-Tetrachloro-isobenzofuran-1,3-dione 4,5,6,7-Tetrachloro-1,3-isobenzofurandione Tetrathal 1,3-Isobenzofurandione, tetrachloro- 1,3-Dioxy-4,5,6,7-tetrachloroisobenzofuran NSC 1484
Inchi:	InChI=1S/C8Cl4O3/c9-3-1-2(8(14)15-7(1)13)4(10)6(12)5(3)11
InchiKey:	AUHHYELHRWCWEZ-UHFFFAOYSA-N
Formula:	C8Cl4O3
SMILES:	O=C1OC(=O)c2c(Cl)c(Cl)c(Cl)c(Cl)c21
Mol. weight [g/mol]:	285.90
CAS:	117-08-8

Physical Properties

Property code	Value	Unit	Source
ea	1.96 ± 0.09	eV	NIST Webbook
gf	-229.82	kJ/mol	Joback Method
hf	-406.49	kJ/mol	Joback Method
hfus	29.42	kJ/mol	Joback Method
hvap	69.75	kJ/mol	Joback Method
ie	10.80 ± 0.20	eV	NIST Webbook
log10ws	-4.67		Crippen Method
logp	3.611		Crippen Method
mcvol	146.930	ml/mol	McGowan Method
pc	3655.35	kPa	Joback Method
rinpol	2029.00		NIST Webbook
rinpol	2029.00		NIST Webbook
tb	644.20	K	NIST Webbook
tc	1032.62	K	Joback Method
tf	573.81	K	Joback Method

vc	0.565	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	293.94	J/mol×K	757.74	Joback Method
cpg	300.95	J/mol×K	803.55	Joback Method
cpg	307.24	J/mol×K	849.37	Joback Method
cpg	312.77	J/mol×K	895.18	Joback Method
cpg	317.48	J/mol×K	940.99	Joback Method
cpg	321.33	J/mol×K	986.81	Joback Method
cpg	324.26	J/mol×K	1032.62	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=C117088&Units=SI

Legend

cpg: Ideal gas heat capacity
ea: Electron affinity
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
ie: Ionization energy
log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
pc: Critical Pressure
rinpol: Non-polar retention indices

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