

# 1,3-Isobenzofurandione, 4,5,6,7-tetrabromo-

<b>Other names:</b>	Phthalic anhydride, tetrabromo- Bromphthal Dion 6692 Firemaster PHT 4 Tetrabromophthalic anhydride 3,4,5,6-Tetrabromophthalic anhydride FG 4000 4,5,6,7-Tetrabromo-1,3-isobenzofurandione Great Lakes PHT4 Saytex RB-49 NSC 4874 PHT 4 Tetrabromophthalic acid anhydride
<b>Inchi:</b>	InChI=1S/C8Br4O3/c9-3-1-2(8(14)15-7(1)13)4(10)6(12)5(3)11
<b>InchiKey:</b>	QHWKHLUUZGSCW-UHFFFAOYSA-N
<b>Formula:</b>	C8Br4O3
<b>SMILES:</b>	O=C1OC(=O)c2c(Br)c(Br)c(Br)c(Br)c21
<b>Mol. weight [g/mol]:</b>	463.70
<b>CAS:</b>	632-79-1

## Physical Properties

Property code	Value	Unit	Source
gf	-124.82	kJ/mol	Joback Method
hf	-238.21	kJ/mol	Joback Method
hfus	33.77	kJ/mol	Joback Method
hvap	77.95	kJ/mol	Joback Method
log10ws	-6.58		Crippen Method
logp	4.047		Crippen Method
mcvol	167.970	ml/mol	McGowan Method
pc	6609.82	kPa	Joback Method
tb	872.66	K	Joback Method
tc	1179.06	K	Joback Method
tf	693.33	K	Joback Method
vc	0.617	m <sup>3</sup> /kmol	Joback Method

# Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	312.32	J/mol×K	872.66	Joback Method
cpg	318.09	J/mol×K	923.73	Joback Method
cpg	323.19	J/mol×K	974.79	Joback Method
cpg	327.64	J/mol×K	1025.86	Joback Method
cpg	331.45	J/mol×K	1076.93	Joback Method
cpg	334.63	J/mol×K	1127.99	Joback Method
cpg	337.19	J/mol×K	1179.06	Joback Method

## Sources

<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</a>
<b>Crippen Method:</b>	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>
<b>Joback Method:</b>	<a href="https://en.wikipedia.org/wiki/Joback_method">https://en.wikipedia.org/wiki/Joback_method</a>
<b>McGowan Method:</b>	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C632791&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C632791&amp;Units=SI</a>

## Legend

<b>cpg:</b>	Ideal gas heat capacity
<b>gf:</b>	Standard Gibbs free energy of formation
<b>hf:</b>	Enthalpy of formation at standard conditions
<b>hfus:</b>	Enthalpy of fusion at standard conditions
<b>hvap:</b>	Enthalpy of vaporization at standard conditions
<b>log10ws:</b>	Log10 of Water solubility in mol/l
<b>logp:</b>	Octanol/Water partition coefficient
<b>mcvol:</b>	McGowan's characteristic volume
<b>pc:</b>	Critical Pressure
<b>tb:</b>	Normal Boiling Point Temperature
<b>tc:</b>	Critical Temperature
<b>tf:</b>	Normal melting (fusion) point
<b>vc:</b>	Critical Volume

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