1,3-Isobenzofurandione, 5,5'-carbonylbis-

Other names:	3,3',4,4'-Benzophenonetetracarboxylic acid dianhydride
	3,3',4,4'-Tetracarboxybenzophenone dianhydride
	3,3',4,4'-benzophenonetetracarboxylic dianhydride
	4,4'-Carbonylbis(phthalic anhydride)
	4,4'-Diphthalic anhydride ketone
	4,4'-carbonyldiphthalic anhydride
	Benzophenone-3,3',4,4'-tetracarboxylic dianhydride
	Benzophenonetetracarboxylic acid anhydride
	Benzophenonetetracarboxylic acid dianhydride
	Benzophenonetetracarboxylic anhydride
	Benzophenonetetracarboxylic dianhydride
	Bis-(3-phthalyl anhydride) ketone
	NSC 78480
	Phthalic anhydride, 4,4'-carbonyldi-
	benzophenone-3,3':4,4'-tetracarboxylic dianhydride
Inchi:	InChI=1S/C17H6O7/c18-13(7-1-3-9-11(5-7)16(21)23-14(9)19)8-2-4-10-12(6-8)17(22)24-1
InchiKey:	VQVIHDPBMFABCQ-UHFFFAOYSA-N
Formula:	C17H6O7
SMILES:	O=C(c1ccc2c(c1)C(=O)OC2=O)c1ccc2c(c1)C(=O)OC2=O
Mol. weight [g/mol]:	322.23
CAS:	2421-28-5

Physical Properties

Property code	Value	Unit	Source
gf	-376.04	kJ/mol	Joback Method
hf	-708.13	kJ/mol	Joback Method
hfus	36.04	kJ/mol	Joback Method
hvap	93.83	kJ/mol	Joback Method
log10ws	-4.34		Crippen Method
logp	1.539		Crippen Method
mcvol	200.740	ml/mol	McGowan Method
pc	3314.37	kPa	Joback Method
ss	350.20	J/mol×K	NIST Webbook
tb	1063.51	K	Joback Method
tc	1353.54	K	Joback Method
tf	804.58	K	Joback Method
vc	0.763	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	627.03	J/mol×K	1305.20	Joback Method
cpg	627.42	J/mol×K	1063.51	Joback Method
cpg	632.07	J/mol×K	1111.85	Joback Method
cpg	634.41	J/mol×K	1160.19	Joback Method
cpg	634.38	J/mol×K	1208.53	Joback Method
cpg	631.94	J/mol×K	1256.86	Joback Method
cpg	619.58	J/mol×K	1353.54	Joback Method
cps	318.70	J/mol×K	300.00	NIST Webbook

Sources

Determining the Solubility of Organic Compounds in Supercritical Carbon Dioxide Using Supercritical Fluid Chromatography Directly Interfaced to Supercritical Fluid Solubility Apparatus:	https://www.doi.org/10.1021/acs.jced.6b00081
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=C2421285&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
cps:	Solid phase 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
ss:	Solid phase molar entropy at standard conditions

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