1,3-Isobenzofurandione, 4-nitro-

Other names:	3-nitro-1,2-benzenedicarboxylic acid anhydride
	3-nitrophthalic anhydride
	Phthalic anhydride, 3-nitro-
Inchi:	InChI=1S/C8H3NO5/c10-7-4-2-1-3-5(9(12)13)6(4)8(11)14-7/h1-3H
InchiKey:	ROFZMKDROVBLNY-UHFFFAOYSA-N
Formula:	C8H3NO5
SMILES:	O=C1OC(=O)c2c1cccc2[N+](=O)[O-]
Mol. weight [g/mol]:	193.11
CAS:	641-70-3

Physical Properties

Property code	Value	Unit	Source
ea	2.05 ± 0.09	eV	NIST Webbook
gf	-117.66	kJ/mol	Joback Method
hf	-319.88	kJ/mol	Joback Method
hfus	25.16	kJ/mol	Joback Method
hvap	66.82	kJ/mol	Joback Method
log10ws	-2.58		Crippen Method
logp	0.905		Crippen Method
mcvol	115.390	ml/mol	McGowan Method
pc	4762.81	kPa	Joback Method
tb	744.92	K	Joback Method
tc	1028.95	K	Joback Method
tf	436.60 ± 0.10	K	NIST Webbook
vc	0.451	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	337.01	J/mol×K	934.27	Joback Method
cpg	342.64	J/mol×K	981.61	Joback Method
cpg	303.96	J/mol×K	744.92	Joback Method
cpg	313.76	J/mol×K	792.26	Joback Method
cpg	322.55	J/mol×K	839.60	Joback Method

cpg	330.30	J/mol×K	886.93	Joback Method
cpg	347.19	J/mol×K	1028.95	Joback Method
hfust	18.40	kJ/mol	436.20	NIST Webbook
hfust	18.40	kJ/mol	436.20	NIST Webbook

Sources

Solid Liquid Equilibria of Ternary 4-Nitro-2-benzofuran-1,3-dione + 3-Nitro-2-benzofuran-1,3-dione + 2-Propanone at 283.15 K and 323.15 K:	https://www.doi.org/10.1021/je301194e
Measurement of Solid Liquid Phase Equilibrium for the Ternary 3-Nitro-2-benzofuran-1,3-dione + 4-Nitrophthalic Anhydride + 1,4-Dioxane System:	https://www.doi.org/10.1021/je500171d
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=C641703&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
ea:	Electron affinity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hfust:	Enthalpy of fusion at a given temperature
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