Benzoic acid, 4-nitro-, anhydride

Other names: p-Nitrobenzoic acid anhydride
Inchi: InChI=1S/C14H8N2O7/c17-13(9-1-5-11(6-2-9)15(19)20)23-14(18)10-3-7-12(8-4-10)16(2
InchiKey: JYMVSZGJZRQOFY-UHFFFAOYSA-N
Formula: C14H8N2O7
SMILES: O=C(OC(=O)c1ccc([N+](=O)[O-])cc1)c1ccc([N+](=O)[O-])cc1
Mol. weight [g/mol]: 316.22
CAS: 902-47-6

Physical Properties

Property code	Value	Unit	Source
gf	-19.18	kJ/mol	Joback Method
hf	-261.07	kJ/mol	Joback Method
hfus	46.43	kJ/mol	Joback Method
hvap	101.72	kJ/mol	Joback Method
log10ws	-4.98		Crippen Method
logp	2.500		Crippen Method
mcvol	204.450	ml/mol	McGowan Method
pc	3096.73	kPa	Joback Method
tb	1016.88	K	Joback Method
tc	1296.07	K	Joback Method
tf	734.73	K	Joback Method
vc	0.797	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	590.04	J/mol×K	1016.88	Joback Method
cpg	596.26	J/mol×K	1063.41	Joback Method
cpg	601.26	J/mol×K	1109.94	Joback Method
cpg	605.12	J/mol×K	1156.48	Joback Method
cpg	607.91	J/mol×K	1203.01	Joback Method
cpg	609.71	J/mol×K	1249.54	Joback Method
cpg	610.59	J/mol×K	1296.07	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C902476&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

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