1,2-Benzenedicarboxylic acid, 3-nitro-

Other names:	3-Nitrophthalic acid
	3-nitro-1,2-benzenedicarboxylic acid
	Phthalic acid, 3-nitro-
	m-Nitrophthalic acid
Inchi:	InChI=1S/C8H5NO6/c10-7(11)4-2-1-3-5(9(14)15)6(4)8(12)13/h1-3H,(H,10,11)(H,12,13)
InchiKey:	KFIRODWJCYBBHY-UHFFFAOYSA-N
Formula:	C8H5NO6
SMILES:	O=C(O)c1cccc([N+](=O)[O-])c1C(=O)O
Mol. weight [g/mol]:	211.13
CAS:	603-11-2

Physical Properties

Property code	Value	Unit	Source
gf	-386.30	kJ/mol	Joback Method
hf	-535.24	kJ/mol	Joback Method
hfus	55.30	kJ/mol	Experimental and computational thermochemistry of 3- and 4-nitrophthalic acids
hvap	100.44	kJ/mol	Joback Method
log10ws	-1.01		Aqueous Solubility Prediction Method
logp	0.991		Crippen Method
mcvol	132.120	ml/mol	McGowan Method
pc	5382.80	kPa	Joback Method
tb	863.02	K	Joback Method
tc	1085.33	K	Joback Method
tf	596.49	K	Joback Method
vc	0.507	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	352.06	J/mol×K	863.02	Joback Method
cpg	357.35	J/mol×K	900.07	Joback Method

cpg	362.11	J/mol×K	937.12	Joback Method
cpg	366.37	J/mol×K	974.18	Joback Method
cpg	370.16	J/mol×K	1011.23	Joback Method
cpg	373.49	J/mol×K	1048.28	Joback Method
cpg	376.40	J/mol×K	1085.33	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C603112&Units=SI
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
Solid-liquid equilibrium (SLE) of ternary system 3-nitrophthalic acid + 4-nitrophthalic acid + 1,4-dioxane at 283.15, 293.15, 303.15, 313.15 and 323.15) K:	https://www.doi.org/10.1016/j.fluid.2013.03.021
Solubility of 3-Nitrophthalic Acid in Different Solvents between 278 K and 298 K:	https://www.doi.org/10.1021/je0604737
Equilibrium Solubility of 3- and 4-Nitrophthalic Acids in Water:	https://www.doi.org/10.1021/je7002594
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
Experimental and computational thermochemistry of 3- and 4-nitrophthalic acids:	https://www.doi.org/10.1016/j.jct.2018.07.026
Solid-liquid phase equilibrium and phase diagram for ternary 3-nitrophthalic acid 4-nitrophthalic acid water system at 283.15K and 333.15K:	https://www.doi.org/10.1016/j.fluid.2007.12.002

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

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