

# 4-nitrophthalic acid

Inchi:	InChI=1S/C8H5NO6/c10-7(11)5-2-1-4(9(14)15)3-6(5)8(12)13/h1-3H,(H,10,11)(H,12,13)
InchiKey:	SLBQXWXKPNIVSQ-UHFFFAOYSA-N
Formula:	C8H5NO6
SMILES:	O=C(O)c1ccc([N+](=O)[O-])cc1C(=O)O
Mol. weight [g/mol]:	211.13

## Physical Properties

Property code	Value	Unit	Source
gf	-386.30	kJ/mol	Joback Method
hf	-535.24	kJ/mol	Joback Method
hfus	37.00	kJ/mol	Experimental and computational thermochemistry of 3- and 4-nitrophthalic acids
hvap	100.44	kJ/mol	Joback Method
log10ws	-2.24		Crippen 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	432.82	K	Research on the application of 7-chloro-quinaldine adducts in 7-chloro-quinaldine separation process
tf	440.00	K	Experimental and computational thermochemistry of 3- and 4-nitrophthalic acids
vc	0.507	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	376.40	J/molxK	1085.33	Joback Method
cpg	366.37	J/molxK	974.18	Joback Method

cpg	362.11	J/molxK	937.12	Joback Method
cpg	357.35	J/molxK	900.07	Joback Method
cpg	352.06	J/molxK	863.02	Joback Method
cpg	370.16	J/molxK	1011.23	Joback Method
cpg	373.49	J/molxK	1048.28	Joback Method
cps	229.53	J/molxK	295.15	Experimental and computational thermochemistry of 3- and 4-nitrophthalic acids
cps	237.97	J/molxK	303.15	Experimental and computational thermochemistry of 3- and 4-nitrophthalic acids
cps	239.13	J/molxK	304.15	Experimental and computational thermochemistry of 3- and 4-nitrophthalic acids
cps	239.66	J/molxK	305.15	Experimental and computational thermochemistry of 3- and 4-nitrophthalic acids
cps	240.19	J/molxK	306.15	Experimental and computational thermochemistry of 3- and 4-nitrophthalic acids
cps	240.50	J/molxK	307.15	Experimental and computational thermochemistry of 3- and 4-nitrophthalic acids
cps	240.61	J/molxK	308.15	Experimental and computational thermochemistry of 3- and 4-nitrophthalic acids
cps	240.93	J/molxK	309.15	Experimental and computational thermochemistry of 3- and 4-nitrophthalic acids
cps	242.51	J/molxK	310.15	Experimental and computational thermochemistry of 3- and 4-nitrophthalic acids

cps	241.24	J/mol×K	311.15	Experimental and computational thermochemistry of 3- and 4-nitrophthalic acids
cps	242.62	J/mol×K	312.15	Experimental and computational thermochemistry of 3- and 4-nitrophthalic acids
cps	243.57	J/mol×K	313.15	Experimental and computational thermochemistry of 3- and 4-nitrophthalic acids
cps	244.09	J/mol×K	314.15	Experimental and computational thermochemistry of 3- and 4-nitrophthalic acids
cps	244.83	J/mol×K	315.15	Experimental and computational thermochemistry of 3- and 4-nitrophthalic acids
cps	245.36	J/mol×K	316.15	Experimental and computational thermochemistry of 3- and 4-nitrophthalic acids
cps	246.10	J/mol×K	317.15	Experimental and computational thermochemistry of 3- and 4-nitrophthalic acids
cps	246.20	J/mol×K	318.15	Experimental and computational thermochemistry of 3- and 4-nitrophthalic acids
cps	246.94	J/mol×K	319.15	Experimental and computational thermochemistry of 3- and 4-nitrophthalic acids
cps	248.00	J/mol×K	320.15	Experimental and computational thermochemistry of 3- and 4-nitrophthalic acids

cps	248.74	J/mol×K	321.15	Experimental and computational thermochemistry of 3- and 4-nitrophthalic acids
cps	249.37	J/mol×K	322.15	Experimental and computational thermochemistry of 3- and 4-nitrophthalic acids
cps	250.22	J/mol×K	323.15	Experimental and computational thermochemistry of 3- and 4-nitrophthalic acids
cps	250.95	J/mol×K	324.15	Experimental and computational thermochemistry of 3- and 4-nitrophthalic acids
cps	251.69	J/mol×K	325.15	Experimental and computational thermochemistry of 3- and 4-nitrophthalic acids
cps	252.22	J/mol×K	326.15	Experimental and computational thermochemistry of 3- and 4-nitrophthalic acids
cps	252.64	J/mol×K	327.15	Experimental and computational thermochemistry of 3- and 4-nitrophthalic acids
cps	253.38	J/mol×K	328.15	Experimental and computational thermochemistry of 3- and 4-nitrophthalic acids
cps	254.02	J/mol×K	329.15	Experimental and computational thermochemistry of 3- and 4-nitrophthalic acids
cps	254.54	J/mol×K	330.15	Experimental and computational thermochemistry of 3- and 4-nitrophthalic acids

cps	255.07	J/mol×K	331.15	Experimental and computational thermochemistry of 3- and 4-nitrophthalic acids
cps	255.71	J/mol×K	332.15	Experimental and computational thermochemistry of 3- and 4-nitrophthalic acids
cps	256.23	J/mol×K	333.15	Experimental and computational thermochemistry of 3- and 4-nitrophthalic acids
cps	256.76	J/mol×K	334.15	Experimental and computational thermochemistry of 3- and 4-nitrophthalic acids
cps	257.50	J/mol×K	335.15	Experimental and computational thermochemistry of 3- and 4-nitrophthalic acids
cps	258.34	J/mol×K	336.15	Experimental and computational thermochemistry of 3- and 4-nitrophthalic acids
cps	256.97	J/mol×K	337.15	Experimental and computational thermochemistry of 3- and 4-nitrophthalic acids
cps	258.45	J/mol×K	338.15	Experimental and computational thermochemistry of 3- and 4-nitrophthalic acids
cps	258.98	J/mol×K	339.15	Experimental and computational thermochemistry of 3- and 4-nitrophthalic acids
cps	259.40	J/mol×K	340.15	Experimental and computational thermochemistry of 3- and 4-nitrophthalic acids

cps	259.93	J/mol×K	341.15	Experimental and computational thermochemistry of 3- and 4-nitrophthalic acids
cps	260.67	J/mol×K	342.15	Experimental and computational thermochemistry of 3- and 4-nitrophthalic acids
cps	261.41	J/mol×K	343.15	Experimental and computational thermochemistry of 3- and 4-nitrophthalic acids
cps	261.72	J/mol×K	344.15	Experimental and computational thermochemistry of 3- and 4-nitrophthalic acids
cps	262.25	J/mol×K	345.15	Experimental and computational thermochemistry of 3- and 4-nitrophthalic acids
cps	262.78	J/mol×K	346.15	Experimental and computational thermochemistry of 3- and 4-nitrophthalic acids
cps	263.52	J/mol×K	347.15	Experimental and computational thermochemistry of 3- and 4-nitrophthalic acids
cps	263.94	J/mol×K	348.15	Experimental and computational thermochemistry of 3- and 4-nitrophthalic acids
cps	264.47	J/mol×K	349.15	Experimental and computational thermochemistry of 3- and 4-nitrophthalic acids
cps	264.99	J/mol×K	350.15	Experimental and computational thermochemistry of 3- and 4-nitrophthalic acids

cps	265.42	J/mol×K	351.15	Experimental and computational thermochemistry of 3- and 4-nitrophthalic acids
cps	266.05	J/mol×K	352.15	Experimental and computational thermochemistry of 3- and 4-nitrophthalic acids
cps	266.26	J/mol×K	353.15	Experimental and computational thermochemistry of 3- and 4-nitrophthalic acids
cps	266.79	J/mol×K	354.15	Experimental and computational thermochemistry of 3- and 4-nitrophthalic acids
cps	267.32	J/mol×K	355.15	Experimental and computational thermochemistry of 3- and 4-nitrophthalic acids
cps	267.74	J/mol×K	356.15	Experimental and computational thermochemistry of 3- and 4-nitrophthalic acids
cps	267.95	J/mol×K	357.15	Experimental and computational thermochemistry of 3- and 4-nitrophthalic acids
cps	268.58	J/mol×K	358.15	Experimental and computational thermochemistry of 3- and 4-nitrophthalic acids
cps	268.90	J/mol×K	359.15	Experimental and computational thermochemistry of 3- and 4-nitrophthalic acids
cps	269.64	J/mol×K	360.15	Experimental and computational thermochemistry of 3- and 4-nitrophthalic acids

cps	269.85	J/mol×K	361.15	Experimental and computational thermochemistry of 3- and 4-nitrophthalic acids
cps	270.27	J/mol×K	362.15	Experimental and computational thermochemistry of 3- and 4-nitrophthalic acids
cps	270.59	J/mol×K	363.15	Experimental and computational thermochemistry of 3- and 4-nitrophthalic acids
cps	271.12	J/mol×K	364.15	Experimental and computational thermochemistry of 3- and 4-nitrophthalic acids
cps	271.86	J/mol×K	365.15	Experimental and computational thermochemistry of 3- and 4-nitrophthalic acids
cps	272.17	J/mol×K	366.15	Experimental and computational thermochemistry of 3- and 4-nitrophthalic acids
cps	272.81	J/mol×K	367.15	Experimental and computational thermochemistry of 3- and 4-nitrophthalic acids
cps	273.23	J/mol×K	368.15	Experimental and computational thermochemistry of 3- and 4-nitrophthalic acids
cps	274.07	J/mol×K	369.15	Experimental and computational thermochemistry of 3- and 4-nitrophthalic acids
cps	274.39	J/mol×K	370.15	Experimental and computational thermochemistry of 3- and 4-nitrophthalic acids

cps	275.02	J/mol×K	371.15	Experimental and computational thermochemistry of 3- and 4-nitrophthalic acids
cps	275.23	J/mol×K	372.15	Experimental and computational thermochemistry of 3- and 4-nitrophthalic acids
cps	275.66	J/mol×K	373.15	Experimental and computational thermochemistry of 3- and 4-nitrophthalic acids
cps	276.29	J/mol×K	374.15	Experimental and computational thermochemistry of 3- and 4-nitrophthalic acids
cps	276.61	J/mol×K	375.15	Experimental and computational thermochemistry of 3- and 4-nitrophthalic acids
cps	277.03	J/mol×K	376.15	Experimental and computational thermochemistry of 3- and 4-nitrophthalic acids
cps	277.56	J/mol×K	377.15	Experimental and computational thermochemistry of 3- and 4-nitrophthalic acids
cps	278.51	J/mol×K	378.15	Experimental and computational thermochemistry of 3- and 4-nitrophthalic acids
cps	279.03	J/mol×K	379.15	Experimental and computational thermochemistry of 3- and 4-nitrophthalic acids
cps	279.56	J/mol×K	380.15	Experimental and computational thermochemistry of 3- and 4-nitrophthalic acids

cps	280.30	J/mol×K	381.15	Experimental and computational thermochemistry of 3- and 4-nitrophthalic acids
cps	280.83	J/mol×K	382.15	Experimental and computational thermochemistry of 3- and 4-nitrophthalic acids
cps	281.57	J/mol×K	383.15	Experimental and computational thermochemistry of 3- and 4-nitrophthalic acids
cps	282.10	J/mol×K	384.15	Experimental and computational thermochemistry of 3- and 4-nitrophthalic acids
cps	282.84	J/mol×K	385.15	Experimental and computational thermochemistry of 3- and 4-nitrophthalic acids
cps	283.26	J/mol×K	386.15	Experimental and computational thermochemistry of 3- and 4-nitrophthalic acids
cps	284.21	J/mol×K	387.15	Experimental and computational thermochemistry of 3- and 4-nitrophthalic acids
cps	284.95	J/mol×K	388.15	Experimental and computational thermochemistry of 3- and 4-nitrophthalic acids
cps	285.37	J/mol×K	389.15	Experimental and computational thermochemistry of 3- and 4-nitrophthalic acids
cps	286.64	J/mol×K	390.15	Experimental and computational thermochemistry of 3- and 4-nitrophthalic acids

cps	237.02	J/mol×K	302.15	Experimental and computational thermochemistry of 3- and 4-nitrophthalic acids
cps	288.22	J/mol×K	392.15	Experimental and computational thermochemistry of 3- and 4-nitrophthalic acids
cps	288.32	J/mol×K	393.15	Experimental and computational thermochemistry of 3- and 4-nitrophthalic acids
cps	289.27	J/mol×K	394.15	Experimental and computational thermochemistry of 3- and 4-nitrophthalic acids
cps	290.33	J/mol×K	395.15	Experimental and computational thermochemistry of 3- and 4-nitrophthalic acids
cps	236.28	J/mol×K	301.15	Experimental and computational thermochemistry of 3- and 4-nitrophthalic acids
cps	234.59	J/mol×K	300.15	Experimental and computational thermochemistry of 3- and 4-nitrophthalic acids
cps	233.22	J/mol×K	299.15	Experimental and computational thermochemistry of 3- and 4-nitrophthalic acids
cps	233.01	J/mol×K	298.15	Experimental and computational thermochemistry of 3- and 4-nitrophthalic acids
cps	232.06	J/mol×K	297.15	Experimental and computational thermochemistry of 3- and 4-nitrophthalic acids

cps	230.90	J/molxK	296.15	Experimental and computational thermochemistry of 3- and 4-nitrophthalic acids
cps	287.48	J/molxK	391.15	Experimental and computational thermochemistry of 3- and 4-nitrophthalic acids
hvapt	114.10	kJ/mol	422.00	Experimental and computational thermochemistry of 3- and 4-nitrophthalic acids
rhos	1647.00	kg/m3	298.15	Experimental and computational thermochemistry of 3- and 4-nitrophthalic acids

## Sources

Research on the application of 7-chloro-quinaldine adducts in 7-chloro-quinaldine separation process:  
McGowan Method:

<https://www.doi.org/10.1016/j.jct.2019.02.002>

[https://en.wikipedia.org/wiki/Joback\\_method](https://en.wikipedia.org/wiki/Joback_method)

<http://link.springer.com/article/10.1007/BF02311772>

Crippen Method:

<http://pubs.acs.org/doi/abs/10.1021/ci990307l>

Crippen Method:

[https://www.chemeo.com/doc/models/crippen\\_log10ws](https://www.chemeo.com/doc/models/crippen_log10ws)

Experimental and computational thermochemistry of 3- and 4-nitrophthalic acids:

<https://www.doi.org/10.1016/j.jct.2018.07.026>

## Legend

<b>cp<sub>g</sub>:</b>	Ideal gas heat capacity
<b>cp<sub>s</sub>:</b>	Solid phase heat capacity
<b>g<sub>f</sub>:</b>	Standard Gibbs free energy of formation
<b>h<sub>f</sub>:</b>	Enthalpy of formation at standard conditions
<b>h<sub>fus</sub>:</b>	Enthalpy of fusion at standard conditions
<b>h<sub>vap</sub>:</b>	Enthalpy of vaporization at standard conditions
<b>h<sub>vapt</sub>:</b>	Enthalpy of vaporization at a given temperature
<b>log<sub>10ws</sub>:</b>	Log10 of Water solubility in mol/l
<b>log<sub>p</sub>:</b>	Octanol/Water partition coefficient

<b>mcvol:</b>	McGowan's characteristic volume
<b>pc:</b>	Critical Pressure
<b>rhos:</b>	Solid Density
<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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