

Benzoic acid, 4-nitro-

Other names:	1-Carboxy-4-nitrobenzene 4-Nitrobenzoic acid 4-Nitrodracylic acid Benzoic acid, p-nitro- Kyselina p-nitrobenzoova NSC 7707 Nitrodracylic acid p-Nitrobenzenecarboxylic acid p-Nitrobenzoic acid p-Nitrodracylic acid p-carboxynitrobenzene
Inchi:	InChI=1S/C7H5NO4/c9-7(10)5-1-3-6(4-2-5)8(11)12/h1-4H,(H,9,10)
InchiKey:	OTLNPYWUJOZPPA-UHFFFAOYSA-N
Formula:	C7H5NO4
SMILES:	O=C(O)c1ccc([N+](=O)[O-])cc1
Mol. weight [g/mol]:	167.12
CAS:	62-23-7

Physical Properties

Property code	Value	Unit	Source
chs	-3049.75	kJ/mol	NIST Webbook
chs	-3042.00 ± 0.80	kJ/mol	NIST Webbook
gf	-119.35	kJ/mol	Joback Method
hf	-238.32	kJ/mol	Joback Method
hfs	-427.20 ± 0.80	kJ/mol	NIST Webbook
hfus	24.59	kJ/mol	Joback Method
hsub	119.70 ± 0.60	kJ/mol	NIST Webbook
hvap	74.13	kJ/mol	Joback Method
ie	10.20 ± 0.20	eV	NIST Webbook
log10ws	-2.75		Aqueous Solubility Prediction Method
logp	1.293		Crippen Method
mvol	110.590	ml/mol	McGowan Method
pc	5051.40	kPa	Joback Method
rinpol	1543.00		NIST Webbook
rinpol	1543.00		NIST Webbook
tb	689.11	K	Joback Method

tc	923.22	K	Joback Method
tf	507.00 ± 3.00	K	NIST Webbook
tf	512.40 ± 0.30	K	NIST Webbook
tf	512.35 ± 0.20	K	NIST Webbook
tf	513.00	K	Solid liquid phase equilibrium and phase diagram for ternary o-nitrobenzoic acid p-nitrobenzoic acid acetone system at 283.15K and 313.15K
tf	513.55	K	Aqueous Solubility Prediction Method
vc	0.426	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	304.86	J/mol×K	923.22	Joback Method
cpg	275.94	J/mol×K	728.13	Joback Method
cpg	282.85	J/mol×K	767.15	Joback Method
cpg	289.17	J/mol×K	806.16	Joback Method
cpg	294.92	J/mol×K	845.18	Joback Method
cpg	300.14	J/mol×K	884.20	Joback Method
cpg	268.39	J/mol×K	689.11	Joback Method
cps	182.80	J/mol×K	297.90	NIST Webbook
cps	197.90	J/mol×K	323.00	NIST Webbook
cps	180.30	J/mol×K	298.00	NIST Webbook
hfust	36.90	kJ/mol	512.40	NIST Webbook
hfust	36.90	kJ/mol	512.40	NIST Webbook
hfust	36.90	kJ/mol	512.35	NIST Webbook
hfust	36.90	kJ/mol	512.40	NIST Webbook
hsubt	115.40 ± 0.60	kJ/mol	374.00	NIST Webbook
sfust	72.00	J/mol×K	512.35	NIST Webbook
sfust	72.00	J/mol×K	512.40	NIST Webbook

Sources

Aqueous Solubility Prediction Method: <http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa>

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

Solubility of p-Nitrobenzoic Acid in Supercritical Carbon Dioxide with and without Cosolvents: <https://www.doi.org/10.1021/je050354b>

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C62237&Units=SI
Solid-Liquid Equilibrium and Phase Diagram for the Ternary p-Nitrobenzoic Acid-m-Nitrobenzoic Acid + Ethanol System:	https://www.doi.org/10.1021/je900364y
Joback Method	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Solid liquid phase equilibrium and phase diagram for ternary system m-nitrobenzoic acid p-nitrobenzoic acid + acetone system at 283.15K and 313.15K	https://www.doi.org/10.1016/j.fluid.2008.02.007
Solid liquid equilibria of the ternary system m-nitrobenzoic acid + p-nitrobenzoic acid + acetone:	https://en.wikipedia.org/wiki/Joback_method
	https://www.doi.org/10.1016/j.fluid.2009.07.011

Legend

chs:	Standard solid enthalpy of combustion
cp_g:	Ideal gas heat capacity
cps:	Solid phase heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfs:	Solid phase enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hfust:	Enthalpy of fusion at a given temperature
hsub:	Enthalpy of sublimation at standard conditions
hsubt:	Enthalpy of sublimation at a given temperature
h_{vap}:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
log₁₀ws:	Log ₁₀ of Water solubility in mol/l
log_p:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
r_{inpol}:	Non-polar retention indices
sfust:	Entropy of fusion at a given temperature
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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