Benzoic acid, 3-nitro-

Other names:	3-Nitrobenzoic acid
	Benzoic acid, m-nitro-
	Metanitrobenzoic acid
	m-Nitrobenzenecarboxylic acid
	m-Nitrobenzoic acid
	m-carboxynitrobenzene
Inchi:	InChI=1S/C7H5NO4/c9-7(10)5-2-1-3-6(4-5)8(11)12/h1-4H,(H,9,10)
InchiKey:	AFPHTEQTJZKQAQ-UHFFFAOYSA-N
Formula:	C7H5NO4
SMILES:	O=C(O)c1cccc([N+](=O)[O-])c1
Mol. weight [g/mol]:	167.12
CAS:	121-92-6

Physical Properties

Property code	Value	Unit	Source
chs	-3053.24	kJ/mol	NIST Webbook
chs	-3055.00 ± 0.40	kJ/mol	NIST Webbook
gf	-119.35	kJ/mol	Joback Method
hf	-238.32	kJ/mol	Joback Method
hfs	-414.00 ± 0.40	kJ/mol	NIST Webbook
hfus	24.59	kJ/mol	Joback Method
hsub	110.00 ± 0.40	kJ/mol	NIST Webbook
hvap	74.13	kJ/mol	Joback Method
ie	10.30 ± 0.20	eV	NIST Webbook
log10ws	-1.72		Aqueous Solubility Prediction Method
logp	1.293		Crippen Method
mcvol	110.590	ml/mol	McGowan Method
pc	5051.40	kPa	Joback Method
tb	689.11	K	Joback Method
tc	923.22	K	Joback Method
tf	414.70	K	Abraham model correlations for describing the thermodynamic properties of solute transfer into pentyl acetate based on headspace chromatographic and solubility measurements

tf	414.90	K	Aqueous Solubility Prediction Method
tf	414.15 ± 1.50	K	NIST Webbook
tf	414.15 ± 1.50	K	NIST Webbook
tf	414.00	K	Solid-Liquid Phase Equilibrium and Phase Diagram for the Ternary o-Nitrobenzoic Acid + m-Nitrobenzoic Acid + Ethanol System
tf	414.30 ± 0.30	K	NIST Webbook
vc	0.426	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	282.85	J/mol×K	767.15	Joback Method
cpg	268.39	J/mol×K	689.11	Joback Method
cpg	275.94	J/mol×K	728.13	Joback Method
cpg	304.86	J/mol×K	923.22	Joback Method
cpg	300.14	J/mol×K	884.20	Joback Method
cpg	294.92	J/mol×K	845.18	Joback Method
cpg	289.17	J/mol×K	806.16	Joback Method
cps	173.20	J/mol×K	298.00	NIST Webbook
cps	201.70	J/mol×K	323.00	NIST Webbook
cps	179.90	J/mol×K	297.90	NIST Webbook
hfust	21.40	kJ/mol	413.00	NIST Webbook
hfust	19.33	kJ/mol	414.30	NIST Webbook
hfust	19.33	kJ/mol	414.30	NIST Webbook
hfust	19.33	kJ/mol	414.30	NIST Webbook
hsubt	107.20 ± 0.40	kJ/mol	354.00	NIST Webbook
sfust	51.60	J/mol×K	413.00	NIST Webbook
sfust	46.70	J/mol×K	414.30	NIST Webbook

Sources

Solubilities of magnesium-L-ascorbate, calcium-L-ascorbate, magnesium-L-glutamate, magnesium-D-gluconate, calcium-D-gluconate, calcium-D-heptagluconate, L-aspartic acid, and 3-nitrobenzoic acid in water:	https://www.doi.org/10.1016/j.jct.2007.12.006
The effect of temperature on the solubility of benzoic acid derivatives in cyclohexane:	https://www.doi.org/10.1016/j.fluid.2006.10.014
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C121926&Units=SI

Binary and ternary solubility of amino- and nitro-benzoic acids in supercritical carbon dioxide:	https://www.doi.org/10.1016/j.fluid.2013.01.021
Solid-Liquid Phase Equilibrium and Phase Diagram for the Ternary o-Nitrobenzoic Acid + m-Nitrobenzoic Acid + Ethanol System:	https://www.doi.org/10.1021/je800080w
Joback Method	https://en.wikipedia.org/wiki/Joback_method
Solid liquid equilibria of the ternary system m-nitrobenzoic acid + p-nitrobenzoic acid + acetone:	https://www.doi.org/10.1016/j.fluid.2009.07.011
Determination and modeling of binary and ternary solid-liquid phase equilibrium for the systems formed by 3,5-dinitrobenzoic acid, m-nitrobenzoic acid and acetone.	https://www.doi.org/10.1016/j.jct.2016.10.004
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
Equilibrium solubility of pure and mixed 3,5-dinitrobenzoic acid and 3-nitrobenzoic acid in supercritical carbon dioxide:	https://www.doi.org/10.1016/j.tca.2011.01.039
Abraham model correlations for describing the thermodynamic properties of solute transfer into pentyl acetate based on headspace chromatographic and solubility measurements:	https://www.doi.org/10.1016/j.jct.2018.05.003
Solid-Liquid Equilibrium and Phase Diagram for the Ternary p-Nitrobenzoic Acid + m-Nitrobenzoic Acid + Ethanol System:	https://www.doi.org/10.1021/je900364y
McGowan Method	http://link.springer.com/article/10.1007/BF02311772

Legend

chs:	Standard solid enthalpy of combustion
cpg:	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
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
sfust:	Entropy of fusion at a given temperature
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume