Benzoic acid, 2-nitro-

Other names:	2-Nitrobenzoic acid
	Benzoic acid, o-nitro-
	o-Nitrobenzoic acid
Inchi:	InChI=1S/C7H5NO4/c9-7(10)5-3-1-2-4-6(5)8(11)12/h1-4H,(H,9,10)
InchiKey:	SLAMLWHELXOEJZ-UHFFFAOYSA-N
Formula:	C7H5NO4
SMILES:	O=C(O)c1ccccc1[N+](=O)[O-]
Mol. weight [g/mol]:	167.12
CAS:	552-16-9

Physical Properties

Property code	Value	Unit	Source
chs	-3077.70	kJ/mol	NIST Webbook
chs	-3071.00 ± 0.63	kJ/mol	NIST Webbook
gf	-119.35	kJ/mol	Joback Method
hf	-238.32	kJ/mol	Joback Method
hfs	-399.00 ± 0.63	kJ/mol	NIST Webbook
hfus	24.59	kJ/mol	Joback Method
hsub	118.70 ± 0.50	kJ/mol	NIST Webbook
hvap	74.13	kJ/mol	Joback Method
log10ws	-1.47		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	419.00 ± 0.30	K	NIST Webbook
tf	420.20	K	Solid-Liquid Phase Equilibrium and Phase Diagram for the Ternary o-Nitrobenzoic Acid + m-Nitrobenzoic Acid + Ethanol System
tf	420.80	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	420.77	K	Aqueous Solubility Prediction Method
vc	0.426	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	300.14	J/mol×K	884.20	Joback Method
cpg	268.39	J/mol×K	689.11	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	304.86	J/mol×K	923.22	Joback Method
cps	190.00	J/mol×K	297.90	NIST Webbook
cps	202.10	J/mol×K	323.00	NIST Webbook
cps	191.60	J/mol×K	298.00	NIST Webbook
hfust	27.99	kJ/mol	419.00	NIST Webbook
hfust	27.99	kJ/mol	419.00	NIST Webbook
hfust	27.99	kJ/mol	419.00	NIST Webbook
hsubt	115.80 ± 0.50	kJ/mol	351.00	NIST Webbook
sfust	66.80	J/mol×K	419.00	NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C552169&Units=SI
Solid liquid phase equilibrium and phase diagram for ternary o-Nitrobenzoic acid p-nitrobenzoic acid acetone system at 283.15K and 318.15K:	https://www.doi.org/10.1016/j.fluid.2008.02.007
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
The effect of temperature on the solubility of benzoic acid derivatives in water:	https://www.doi.org/10.1016/j.fluid.2006.10.014
Solubility of o-Nitrobenzoic Acid in Modified Supercritical Carbon Dioxide at (308 to 328) K:	https://www.doi.org/10.1021/je300023v
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
Solubilities of Benzoic Acid, p-Methylbenzoic Acid, m-Methylbenzoic Acid, o-Methylbenzoic Acid, p-Hydroxybenzoic Acid, and o-Nitrobenzoic Acid in 1-Octanol:	https://www.doi.org/10.1021/je700677d
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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
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