Benzamide, 4-nitro-

Other names:	4-Nitrobenzamide
	Benzamide, p-nitro-
	p-Nitrobenzamide
Inchi:	InChI=1S/C7H6N2O3/c8-7(10)5-1-3-6(4-2-5)9(11)12/h1-4H,(H2,8,10)
InchiKey:	ZESWUEBPRPGMTP-UHFFFAOYSA-N
Formula:	C7H6N2O3
SMILES:	NC(=O)c1ccc([N+](=O)[O-])cc1
Mol. weight [g/mol]:	166.13
CAS:	619-80-7

Physical Properties

Property code	Value	Unit	Source
affp	845.30	kJ/mol	NIST Webbook
basg	814.40	kJ/mol	NIST Webbook
gf	83.92	kJ/mol	Joback Method
hf	-52.30	kJ/mol	Joback Method
hfus	30.09	kJ/mol	Gas phase enthalpies of formation of nitrobenzamides using combustion calorimetry and thermal analysis
hvap	68.09	kJ/mol	Joback Method
ie	10.33	eV	NIST Webbook
log10ws	-2.29		Crippen Method
logp	0.694		Crippen Method
mcvol	114.700	ml/mol	McGowan Method
pc	4809.16	kPa	Joback Method
tb	669.46	K	Joback Method
tc	933.02	K	Joback Method
tf	484.39	K	Joback Method
tt	473.45	K	Solubility Determination and Modeling of p-Nitrobenzamide Dissolved in Twelve Neat Solvents from 283.15 to 328.15 K
vc	0.436	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	278.75	J/mol×K	669.46	Joback Method
cpg	288.09	J/mol×K	713.39	Joback Method
cpg	296.56	J/mol×K	757.31	Joback Method
cpg	304.23	J/mol×K	801.24	Joback Method
cpg	311.14	J/mol×K	845.17	Joback Method
cpg	317.33	J/mol×K	889.09	Joback Method
cpg	322.86	J/mol×K	933.02	Joback Method

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Gas phase enthalpies of formation of nitrobenzamides using combustion calorimetry and thermal analysis:	https://www.doi.org/10.1016/j.jct.2014.07.006
Thermodynamic solubility modelling, solvent effect and preferential solvation of p-nitrobenzamide in aqueous co-solvent mixtures of dimethyl sulfoxide, ethanol, isopropanol and propylene glycol:	https://www.doi.org/10.1016/j.jct.2019.05.007
Solubility Determination and Modeling of p-Nitrobenzamide Dissolved in Various Neat Solvents from 283.15 to 328.15 K:	https://www.doi.org/10.1021/acs.jced.9b00065
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C619807&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

affp:	Proton affinity
basg:	Gas basicity
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
ie:	Ionization energy
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
tt:	Triple Point Temperature
vc:	Critical Volume