P-NITROBENZAMIDE

Other names:	4-Nitrobenzamide
	Benzamide, p-nitro-
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]:	166.14

Physical Properties

Property code	Value	Unit	Source
affp	845.30	kJ/mol	NIST Webbook
basg	814.40	kJ/mol	NIST Webbook
hf	-129.15	kJ/mol	Cheméo Relay (1.0)
hfus	30.09	kJ/mol	Gas phase enthalpies of formation of nitrobenzamides using combustion calorimetry and thermal analysis
hvap	87.39	kJ/mol	Cheméo Relay (1.0)
ie	10.33	eV	NIST Webbook
log10ws	-2.62		Cheméo Relay (1.0)
logp	0.694		Crippen Method
mcvol	114.700	ml/mol	McGowan Method
tb	559.41	K	Cheméo Relay (1.0)
tf	444.60	K	Cheméo Relay (1.0)
tt	473.45	K	Solubility Determination and Modeling of p-Nitrobenzamide Dissolved in Twelve Neat Solvents from 283.15 to 328.15 K

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

Cheméo Relay (1.0, beta):

Solubility Determination and Modeling of p-Nitrobenzamide Dissolved in Twelve Neat Solvents from 283.15 to 328.15 K: https://www.doi.org/10.1021/acs.jced.9b00065

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Thermodynamic solubility modelling, solvent effect and preferential solvation of p-nitrobenzamide in aqueous co-solvent mixtures of dimethyl sulfoxide, ethanol, isopropanol and ethyl acetate: https://www.doi.org/10.1016/j.jct.2019.05.007

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C619807&Units=SI

Gas phase enthalpies of formation of nitrobenzamides using combustion calorimetry and thermal analysis: https://www.doi.org/10.1016/j.jct.2014.07.006

Joback Method: https://en.wikipedia.org/wiki/Joback_method

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Cheméo Relay (1.0):

Estimation of sublimation enthalpies of aromatic amides at 298.15 K from the values of fusion enthalpies: https://www.doi.org/10.1016/j.tca.2016.10.015

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

Legend

affp:	Proton affinity
basg:	Gas basicity
cpg:	Ideal gas heat capacity
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
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point
tt:	Triple Point Temperature

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