4-Nitrobenzoic hydrazide

Other names:	(4-Nitrobenzoyl)hydrazide
	(4-Nitrobenzoyl)hydrazine
	(p-Nitrobenzoyl)hydrazine
	4-Nitrobenzhydrazide
	4-Nitrobenzohydrazide
	4-Nitrobenzoic acid hydrazide
	Benzoic acid, 4-nitro-, hydrazide
	Benzoic acid, p-nitro-, hydrazide
	NSC 9804
	p-Nitrobenzhydrazide
	p-Nitrobenzohydrazide
	p-Nitrobenzoic acid hydrazide
	p-Nitrobenzoic hydrazide
	p-Nitrobenzoylhydrazide
Inchi:	InChI=1S/C7H7N3O3/c8-9-7(11)5-1-3-6(4-2-5)10(12)13/h1-4H,8H2,(H,9,11)
InchiKey:	FKZXYJYTUSGIQE-UHFFFAOYSA-N
Formula:	C7H7N3O3
SMILES:	NNC(=O)c1ccc([N+](=O)[O-])cc1
Mol. weight [g/mol]:	181.15
CAS:	636-97-5

Physical Properties

Property code	Value	Unit	Source
gf	173.31	kJ/mol	Joback Method
hf	1.17	kJ/mol	Joback Method
hfus	30.79	kJ/mol	Joback Method
hvap	74.53	kJ/mol	Joback Method
log10ws	-2.16		Aqueous Solubility Prediction Method
logp	0.198		Crippen Method
mcvol	124.680	ml/mol	McGowan Method
pc	4897.06	kPa	Joback Method
tb	719.63	K	Joback Method
tc	978.77	K	Joback Method
tf	537.05	K	Joback Method
vc	0.471	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	321.71	J/mol×K	719.63	Joback Method
cpg	330.87	J/mol×K	762.82	Joback Method
cpg	339.15	J/mol×K	806.01	Joback Method
cpg	346.62	J/mol×K	849.20	Joback Method
cpg	353.32	J/mol×K	892.39	Joback Method
cpg	359.30	J/mol×K	935.58	Joback Method
cpg	364.62	J/mol×K	978.77	Joback Method

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Joback Method: https://en.wikipedia.org/wiki/Joback_method
Aqueous Solubility Prediction Method: http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C636975&Units=SI

Legend

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
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
vc: Critical Volume