Acetamide, N-(4-nitrophenyl)-

Other names:	1-Nitro-4-acetylaminobenzene
	4'-Nitroacetanilide
	4-(Acetylamino)nitrobenzene
	4-Nitroacetanilide
	Acetanilide, 4'-nitro-
	Acetanilide, p-nitro-
	N-(4-Nitrophenyl)acetamide
	N-(4-Nitrophenyl)acetic acid amide
	N-(p-Nitrophenyl)acetamide
	N-Acetyl-4-nitroaniline
	N-Acetyl-4-nitrobenzenamine
	N-Acetyl-p-nitroaniline
	NSC 1315
	p-Acetamidonitrobenzene
	p-Nitroacetanilide
	p-Nitrophenylacetanilide
Inchi:	InChI=1S/C8H8N2O3/c1-6(11)9-7-2-4-8(5-3-7)10(12)13/h2-5H,1H3,(H,9,11)
InchiKey:	NQRLPDFELNCFHW-UHFFFAOYSA-N
Formula:	C8H8N2O3
SMILES:	CC(=O)Nc1ccc([N+](=O)[O-])cc1
Mol. weight [g/mol]:	180.16
CAS:	104-04-1

Physical Properties

Property code	Value	Unit	Source
gf	115.28	kJ/mol	Joback Method
hf	-53.26	kJ/mol	Joback Method
hfus	28.19	kJ/mol	Joback Method
hvap	66.11	kJ/mol	Joback Method
ie	9.10 ± 0.20	eV	NIST Webbook
log10ws	-2.69		Estimated Solubility Method
log10ws	-2.69		Aqueous Solubility Prediction Method
logp	1.553		Crippen Method
mcvol	128.790	ml/mol	McGowan Method
pc	3995.65	kPa	Joback Method

tb	669.98	K	Joback Method
tc	918.65	K	Joback Method
tf	488.82	K	Aqueous Solubility Prediction Method
tf	489.10 ± 0.10	K	NIST Webbook
vc	0.498	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	320.18	J/mol×K	669.98	Joback Method
cpg	330.79	J/mol×K	711.43	Joback Method
cpg	340.52	J/mol×K	752.87	Joback Method
cpg	349.41	J/mol×K	794.32	Joback Method
cpg	357.50	J/mol×K	835.76	Joback Method
cpg	364.84	J/mol×K	877.21	Joback Method
cpg	371.48	J/mol×K	918.65	Joback Method
cps	230.50	J/mol×K	323.00	NIST Webbook

Sources

Joback Method: https://en.wikipedia.org/wiki/Joback_method
Aqueous Solubility Prediction Method: http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
Estimated Solubility Method: http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C104041&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

cpg: Ideal gas heat capacity
cps: Solid phase 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
vc:	Critical Volume

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