Acetamide, N-(4-aminophenyl)-

Other names:	1-Amino-4-(acetylamino)benzene
	4'-Aminoacetanilid
	4'-Aminoacetanilide
	4-(Acetylamino)aniline
	4-Acetamidoaniline
	4-Acetoamidoaniline
	4-Aminoacetanilide
	Acetanilide, 4'-amino-
	Acetparamin
	Acetyl-p-phenylenediamine
	C.I. 76005
	C.I. Oxidation Base 19
	Fourrine 88
	Fourrine A
	N-(4-Aminophenyl)acetamide
	N-(p-Aminophenyl)acetamide
	N-Acetyl-1,4-benzenediamine
	N-Acetyl-p-fenylendiamin
	N-Acetyl-p-phenylenediamine
	NSC 2135
	Paracetamin
	p-(Acetylamino)aniline
	p-Acetamidoaniline
	p-Acetaminoaniline
	p-Acetoaminoaniline
	p-Aminoacetanilide
Inchi:	InChI=1S/C8H10N2O/c1-6(11)10-8-4-2-7(9)3-5-8/h2-5H,9H2,1H3,(H,10,11)
InchiKey:	CHMBIJAOCISYEW-UHFFFAOYSA-N
Formula:	C8H10N2O
SMILES:	CC(=O)Nc1ccc(N)cc1
Mol. weight [g/mol]:	150.18
CAS:	122-80-5

Physical Properties

Property code	Value	Unit	Source
gf	146.18	kJ/mol	Joback Method

hf	-8.71	kJ/mol	Joback Method
hfus	22.02	kJ/mol	Joback Method
hvap	60.16	kJ/mol	Joback Method
ie	7.12 ± 0.02	eV	NIST Webbook
log10ws	-0.98		Aqueous Solubility Prediction Method
logp	1.227		Crippen Method
mcvol	121.350	ml/mol	McGowan Method
pc	4233.04	kPa	Joback Method
tb	590.67	K	Joback Method
tc	823.28	K	Joback Method
tf	437.90	K	Aqueous Solubility Prediction Method
vc	0.446	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	286.50	J/mol×K	590.67	Joback Method
cpg	297.98	J/mol×K	629.44	Joback Method
cpg	308.67	J/mol×K	668.21	Joback Method
cpg	318.60	J/mol×K	706.98	Joback Method
cpg	327.79	J/mol×K	745.75	Joback Method
cpg	336.28	J/mol×K	784.52	Joback Method
cpg	344.12	J/mol×K	823.28	Joback Method

Sources

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=C122805&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Joback Method: https://en.wikipedia.org/wiki/Joback_method

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
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