

Phenol, 4-amino-

Other names:	1-Amino-4-hydroxybenzene
	4-Amino-1-hydroxybenzene
	4-Aminobenzenol
	4-Aminophenol
	4-Hydroxyaniline
	4-hydroxy-1-aminobenzene
	4-hydroxybenzenamine
	4-hydroxyphenylamine
	Activol
	Azol
	BASF Ursol P Base
	Benzofur P
	C.I. 76550
	C.I. Oxidation Base 6
	C.I. Oxidation Base 6A
	Certinal
	Citol
	Durafur Brown RB
	Fouramine P
	Fourrine 84
	Fourrine P Base
	Furro P base
	Kodelon
	NSC 1545
	Nako Brown R
	PAP
	Para-aminophenol
	Paramidophenol
	Paranol
	Pelagol Grey P Base
	Pelagol P Base
	Phenol, p-amino-
	Renal AC
	Rodinal
	Takatol
	Tertral P Base
	UN 2512
	Unal
	Ursol P
	Ursol P Base

Zoba Brown P Base
p-Aminofenol
p-Aminophenol
p-Hydroxyaniline
p-Hydroxyphenylamine

Inchi: InChI=1S/C6H7NO/c7-5-1-3-6(8)4-2-5/h1-4,8H,7H2
InchiKey: PLIKAWJENQZMHA-UHFFFAOYSA-N
Formula: C6H7NO
SMILES: Nc1ccc(O)cc1
Mol. weight [g/mol]: 109.13
CAS: 123-30-8

Physical Properties

Property code	Value	Unit	Source
chs	-3194.00	kJ/mol	NIST Webbook
chs	-3167.40 ± 0.90	kJ/mol	NIST Webbook
chs	-3170.90 ± 0.50	kJ/mol	NIST Webbook
gf	23.88	kJ/mol	Joback Method
hf	-81.50 ± 1.70	kJ/mol	NIST Webbook
hf	-90.50 ± 1.20	kJ/mol	NIST Webbook
hfs	-194.10	kJ/mol	NIST Webbook
hfs	-168.00	kJ/mol	NIST Webbook
hfs	-190.60 ± 0.90	kJ/mol	NIST Webbook
hfus	16.32	kJ/mol	Joback Method
hsub	109.10 ± 1.40	kJ/mol	NIST Webbook
hsub	109.10 ± 1.40	kJ/mol	NIST Webbook
hsub	103.60 ± 0.70	kJ/mol	NIST Webbook
hsub	103.63 ± 0.65	kJ/mol	NIST Webbook
hvap	54.88	kJ/mol	Joback Method
log10ws	-0.80		Estimated Solubility Method
log10ws	-0.80		Aqueous Solubility Prediction Method
logp	0.974		Crippen Method
mcvol	87.490	ml/mol	McGowan Method
pc	6328.92	kPa	Joback Method
rinpol	1265.00		NIST Webbook
rinpol	1314.00		NIST Webbook
rinpol	1265.00		NIST Webbook
rinpol	1265.00		NIST Webbook
rinpol	1314.00		NIST Webbook

rmpol	1314.00		NIST Webbook
rmpol	1314.00		NIST Webbook
tb	516.51	K	Joback Method
tc	762.01	K	Joback Method
tf	459.50 ± 0.50	K	NIST Webbook
tf	462.50 ± 1.00	K	NIST Webbook
tf	461.53	K	Aqueous Solubility Prediction Method
tf	463.40 ± 1.00	K	NIST Webbook
tf	465.00 ± 2.00	K	NIST Webbook
tf	457.00 ± 0.20	K	NIST Webbook
vc	0.259	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	224.18	J/mol×K	680.18	Joback Method
cpg	236.99	J/mol×K	762.01	Joback Method
cpg	230.81	J/mol×K	721.09	Joback Method
cpg	191.19	J/mol×K	516.51	Joback Method
cpg	200.59	J/mol×K	557.43	Joback Method
cpg	209.16	J/mol×K	598.34	Joback Method
cpg	217.00	J/mol×K	639.26	Joback Method
hfust	26.00	kJ/mol	462.50	NIST Webbook
hfust	23.80	kJ/mol	455.20	NIST Webbook
hfust	31.20	kJ/mol	459.50	NIST Webbook
hsubt	92.10	kJ/mol	416.50	NIST Webbook
hsubt	111.00	kJ/mol	441.00	NIST Webbook
hsubt	101.10 ± 0.70	kJ/mol	335.00	NIST Webbook

Sources

Crippen Method:

<http://pubs.acs.org/doi/abs/10.1021/ci990307l>

Solubilities of p-Aminophenol in Sulfuric acid + Water from (286.15 to 323.15) K: and Viscosities of p-Aminophenol in Sulfuric Acid + Water at Temperatures from (293.15 to 343.15) K:

<https://www.doi.org/10.1021/je049552d>
<https://www.doi.org/10.1021/je050443o>
https://en.wikipedia.org/wiki/Joback_method

Aqueous Solubility Prediction Method:

<http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDataset002.xlsx>

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=C123308&Units=SI>

Legend

chs:	Standard solid enthalpy of combustion
cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfs:	Solid phase enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hfust:	Enthalpy of fusion at a given temperature
hsub:	Enthalpy of sublimation at standard conditions
hsubt:	Enthalpy of sublimation at a given temperature
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
rinpola:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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