

Phenol, 2-amino-

Other names:	1-amino-2-hydroxybenzene
	1-hydroxy-2-aminobenzene
	2-Amino-1-hydroxybenzene
	2-Aminophenyl alcohol
	2-Hydroxyaniline
	2-aminophenol
	2-hydroxyaniline
	2-hydroxybenzenamine
	BASF Ursol 3GA
	Benzene, 1-hydroxy-2-amine-
	Benzofur GG
	C.I. 76520
	C.I. Oxidation Base 17
	Fouramine OP
	NSC 1534
	Nako Yellow 3GA
	Nako Yellow ga
	Paradone Olive Green B
	Pelagol 3GA
	Pelagol Grey GG
	Questionmycin B
	Zoba 3GA
	o-aminohydroxybenzene
	o-aminophenol
	o-hydroxyaniline
	o-hydroxyphenylamine
	phenol, o-amino-
Inchi:	InChI=1S/C6H7NO/c7-5-3-1-2-4-6(5)8/h1-4,8H,7H2
InchiKey:	CDAWCLOXVUBKRW-UHFFFAOYSA-N
Formula:	C6H7NO
SMILES:	Nc1ccccc1O
Mol. weight [g/mol]:	109.13

Physical Properties

Property code	Value	Unit	Source
af	0.5860		Cheméo Relay (1.0)

affp	898.80	kJ/mol	NIST Webbook
basg	866.90	kJ/mol	NIST Webbook
chs	-3170.50 ± 0.50	kJ/mol	NIST Webbook
chs	-3160.10 ± 1.50	kJ/mol	NIST Webbook
gf	23.88	kJ/mol	Joback Method
hf	-104.40 ± 1.70	kJ/mol	NIST Webbook
hf	-87.10 ± 1.30	kJ/mol	NIST Webbook
hfs	-201.30 ± 1.50	kJ/mol	NIST Webbook
hfs	-191.00 ± 0.90	kJ/mol	NIST Webbook
hfus	16.32	kJ/mol	Joback Method
hsub	96.90 ± 0.60	kJ/mol	NIST Webbook
hsub	103.90 ± 0.90	kJ/mol	NIST Webbook
hsub	103.90 ± 0.90	kJ/mol	NIST Webbook
hsub	96.90 ± 0.60	kJ/mol	NIST Webbook
hvap	66.21	kJ/mol	Cheméo Relay (1.0)
ie	7.66	eV	Cheméo Relay (1.0)
log10ws	-0.72		Estimated Solubility Method
log10ws	-0.72		Aqueous Solubility Prediction Method
logp	0.974		Crippen Method
mcvol	87.490	ml/mol	McGowan Method
pc	6328.92	kPa	Joback Method
rinpol	1251.00		NIST Webbook
rinpol	1242.00		NIST Webbook
rinpol	1242.00		NIST Webbook
rinpol	1251.00		NIST Webbook
tb	527.54	K	Cheméo Relay (1.0)
tc	781.18	K	Cheméo Relay (1.0)
tf	447.53	K	Vapour pressures and thermodynamic stability of the three aminophenol isomers
tf	447.90	K	Aqueous Solubility Prediction Method
tf	447.40 ± 0.50	K	NIST Webbook
tf	446.70 ± 0.20	K	NIST Webbook
tf	448.72	K	Thermodynamic study of solvent-free reaction between 17-methyltestosterone and o-aminophenol
vc	0.291	m ³ /kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
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
cpg	224.18	J/mol×K	680.18	Joback Method
cpg	230.81	J/mol×K	721.09	Joback Method
cpg	236.99	J/mol×K	762.01	Joback Method
hfust	21.72	kJ/mol	447.60	NIST Webbook
hfust	31.40	kJ/mol	443.20	NIST Webbook
hfust	34.00	kJ/mol	447.40	NIST Webbook
hsubt	93.50 ± 0.80	kJ/mol	332.00	NIST Webbook
hsubt	95.30 ± 0.70	kJ/mol	337.00	NIST Webbook

Sources

Heat capacities of aqueous polar aromatic compounds over a wide range of temperatures. Part II: dihydroxybenzenes, aminophenols, diamino benzenes, and thermodynamic stability of the three aminophenol isomers

<https://www.doi.org/10.1016/j.jct.2004.09.001>

Cheméo Relay (1.0, beta):

Estimated Solubility Method:

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

<https://www.doi.org/10.1016/j.jct.2018.09.011>

<http://link.springer.com/article/10.1007/BF02311772>

Cheméo Relay (1.0):

Thermodynamic study of solvent-free reaction between Anilines, Resubstituted and o-aminophenol:

<https://www.doi.org/10.1016/j.jct.2011.02.003>

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

<http://webbook.nist.gov/cgi/cbook.cgi?ID=C95556&Units=SI>

Joback Method:

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

Legend

af: Acentric Factor
affp: Proton affinity
basg: Gas basicity
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
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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