Phenol, 3-amino-

Other names:	1-amino-3-hydroxybenzene
	3-Amino-1-hydroxybenzene
	3-aminophenol
	3-hydroxyaniline
	3-hydroxybenzenamine
	Basf ursol eg
	C.I. 76545
	C.I. Oxidation Base 7
	Fouramine EG
	Fourrine 65
	Fourrine EG
	Furro EG
	Futramine EG
	NSC 1546
	Nako TEG
	Pelagol EG
	Renal EG
	Tertral EG
	Ursol EG
	Zoba EG
	m-Aminofenol
	m-aminophenol
	m-hydroxyaminobenzene
	m-hydroxyaniline
	m-hydroxyphenylamine
	phenol, m-amino-
Inchi:	InChI=1S/C6H7NO/c7-5-2-1-3-6(8)4-5/h1-4,8H,7H2
InchiKey:	CWLKGDAVCFYWJK-UHFFFAOYSA-N
Formula:	C6H7NO
SMILES:	Nc1cccc(O)c1
Mol. weight [g/mol]:	109.13
CAS:	591-27-5

Physical Properties

Property code	Value	Unit	Source
affp	898.80	kJ/mol	NIST Webbook

basg	866.90	kJ/mol	NIST Webbook
chs	-3167.40 ± 0.60	kJ/mol	NIST Webbook
chs	-3161.20 ± 1.20	kJ/mol	NIST Webbook
gf	23.88	kJ/mol	Joback Method
hf	-89.40 ± 1.60	kJ/mol	NIST Webbook
hf	-98.60 ± 1.60	kJ/mol	NIST Webbook
hfs	-200.20 ± 1.20	kJ/mol	NIST Webbook
hfs	-194.10 ± 1.00	kJ/mol	NIST Webbook
hfus	27.60	kJ/mol	Synthesis and characterization of novel binary organic monotectic and eutectic alloys
hsub	104.70 ± 1.20	kJ/mol	NIST Webbook
hsub	101.60 ± 0.90	kJ/mol	NIST Webbook
hsub	104.70 ± 1.20	kJ/mol	NIST Webbook
hsub	101.60 ± 0.90	kJ/mol	NIST Webbook
hvap	54.88	kJ/mol	Joback Method
log10ws	-0.65		Crippen Method
logp	0.974		Crippen Method
mcvol	87.490	ml/mol	McGowan Method
pc	6328.92	kPa	Joback Method
rinpol	1335.00		NIST Webbook
rinpol	1335.00		NIST Webbook
rinpol	1335.00		NIST Webbook
rinpol	1335.00		NIST Webbook
tb	516.51	K	Joback Method
tc	762.01	K	Joback Method
tf	396.00 ± 0.20	K	NIST Webbook
tf	398.00 ± 1.00	K	NIST Webbook
tf	394.00 ± 0.50	K	NIST Webbook
vc	0.259	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	236.99	J/mol×K	762.01	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	191.19	J/mol×K	516.51	Joback Method

hfust	22.97	kJ/mol	396.00	NIST Webbook
hfust	21.95	kJ/mol	396.80	NIST Webbook
hfust	23.90	kJ/mol	390.70	NIST Webbook
hfust	22.98	kJ/mol	399.00	NIST Webbook
hfust	22.98	kJ/mol	399.00	NIST Webbook
hsubt	98.80 ± 0.90	kJ/mol	335.00	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	437.20	K	1.50	NIST Webbook
tbrp	437.00	K	1.50	NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C591275&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Synthesis and characterization of novel binary organic monotectic and eutectic alloys:	https://www.doi.org/10.1016/j.tca.2012.02.020
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

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
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
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume