p-Aminotoluene

Other names:	1-Amino-4-methylbenzene
	4-Amino-1-methylbenzene
	4-Aminotoluen
	4-Aminotoluene
	4-METHYLBENZENEAMINE
	4-Methylaniline
	4-Methylbenzenamine
	4-Toluidine
	4-Tolylamine
	Aniline, p-methyl-
	Benzenamine, 4-methyl-
	C.I. 37107
	C.I. Azoic coupling component 107
	NSC 15350
	Naphtol AS-KG
	Naphtol AS-KGLL
	P-METHYLANILINE
	Rcra waste number U353
	p-Methylbenzenamine
	p-Toluidin
	p-Toluidine
	p-Tolylamine
Inchi:	InChI=1S/C7H9N/c1-6-2-4-7(8)5-3-6/h2-5H,8H2,1H3
InchiKey:	RZXMPPFPUUCRFN-UHFFFAOYSA-N
Formula:	C7H9N
SMILES:	Cc1ccc(N)cc1
Mol. weight [g/mol]:	107.15
CAS:	106-49-0

Physical Properties

Property code	Value	Unit	Source
af	0.4430		KDB
affp	896.70	kJ/mol	NIST Webbook
basg	864.80	kJ/mol	NIST Webbook
chl	-4059.00	kJ/mol	NIST Webbook
chl	-4061.40	kJ/mol	NIST Webbook

dm	1.60	debye	KDB
gf	177.29	kJ/mol	Joback Method
hf	62.20	kJ/mol	NIST Webbook
hf	41.80	kJ/mol	NIST Webbook
hfl	19.00	kJ/mol	NIST Webbook
hfus	12.73	kJ/mol	Joback Method
hsub	76.20 ± 0.30	kJ/mol	NIST Webbook
hsub	78.80 ± 0.50	kJ/mol	NIST Webbook
hvap	62.10	kJ/mol	NIST Webbook
hvap	57.80 ± 0.30	kJ/mol	NIST Webbook
hvap	55.90	kJ/mol	NIST Webbook
hvap	43.18	kJ/mol	NIST Webbook
ie	7.65	eV	NIST Webbook
ie	7.24 ± 0.02	eV	NIST Webbook
ie	7.37	eV	NIST Webbook
ie	7.60 ± 0.10	eV	NIST Webbook
ie	7.60 ± 0.10	eV	NIST Webbook
ie	7.85 ± 0.05	eV	NIST Webbook
ie	7.78	eV	NIST Webbook
ie	7.58	eV	NIST Webbook
ie	7.81	eV	NIST Webbook
ie	7.62	eV	NIST Webbook
log10ws	-1.21		Estimated Solubility Method
log10ws	-1.21		Aqueous Solubility Prediction Method
logp	1.577		Crippen Method
mcvol	95.710	ml/mol	McGowan Method
pc	2381.14 ± 202.65	kPa	NIST Webbook
pc	4580.00	kPa	KDB
rinpol	1042.10		NIST Webbook
rinpol	1068.00		NIST Webbook
rinpol	1073.00		NIST Webbook
rinpol	1092.00		NIST Webbook
rinpol	1056.50		NIST Webbook
rinpol	1037.00		NIST Webbook
rinpol	176.89		NIST Webbook
rinpol	1042.10		NIST Webbook
rinpol	1068.00		NIST Webbook
rinpol	1092.00		NIST Webbook
ripol	1839.00		NIST Webbook
ripol	1836.10		NIST Webbook
ripol	1828.90		NIST Webbook
ripol	1822.00		NIST Webbook
ripol	1825.00		NIST Webbook

ripol	1833.90		NIST Webbook
ripol	1822.00		NIST Webbook
ripol	1836.10		NIST Webbook
ripol	1828.90		NIST Webbook
ripol	1822.00		NIST Webbook
tb	475.70 ± 1.00	K	NIST Webbook
tb	473.70 ± 0.30	K	NIST Webbook
tb	473.70	K	NIST Webbook
tb	473.57	K	KDB
tb	473.65 ± 0.30	K	NIST Webbook
tb	473.65 ± 0.30	K	NIST Webbook
tb	473.70 ± 0.30	K	NIST Webbook
tb	473.50 ± 0.20	K	NIST Webbook
tb	473.45 ± 0.60	K	NIST Webbook
tb	473.65 ± 0.50	K	NIST Webbook
tc	706.00	K	KDB
tc	667.15 ± 2.00	K	NIST Webbook
tf	317.15 ± 0.50	K	NIST Webbook
tf	318.70 ± 0.20	K	NIST Webbook
tf	317.00 ± 0.20	K	NIST Webbook
tf	316.95 ± 0.30	K	NIST Webbook
tf	316.90	K	KDB
tf	316.85 ± 0.40	K	NIST Webbook
tf	316.40 ± 2.00	K	NIST Webbook
tf	317.40 ± 0.60	K	NIST Webbook
tf	316.90 ± 0.10	K	NIST Webbook
tf	316.80	K	Aqueous Solubility Prediction Method
tf	316.70 ± 0.50	K	NIST Webbook
tf	316.15 ± 0.30	K	NIST Webbook
tf	318.15 ± 1.50	K	NIST Webbook
tf	315.60 ± 1.00	K	NIST Webbook
tf	318.15 ± 1.50	K	NIST Webbook
tf	315.95 ± 0.50	K	NIST Webbook
tf	318.00 ± 1.50	K	NIST Webbook
tf	313.30 ± 0.05	K	NIST Webbook
tf	316.55 ± 0.50	K	NIST Webbook
tf	318.00 ± 1.50	K	NIST Webbook
tf	318.15 ± 1.00	K	NIST Webbook
tf	318.15 ± 1.50	K	NIST Webbook
tf	316.85 ± 0.30	K	NIST Webbook
tf	316.15 ± 0.50	K	NIST Webbook
tf	316.65 ± 0.30	K	NIST Webbook
tf	316.65 ± 0.50	K	NIST Webbook
tf	316.80 ± 0.40	K	NIST Webbook

tf	316.55 ± 0.40	K	NIST Webbook
vc	0.348	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	188.04	J/mol×K	463.75	Joback Method
cpg	199.40	J/mol×K	501.76	Joback Method
cpg	210.07	J/mol×K	539.77	Joback Method
cpg	220.08	J/mol×K	577.78	Joback Method
cpg	229.46	J/mol×K	615.79	Joback Method
cpg	238.23	J/mol×K	653.80	Joback Method
cpg	246.42	J/mol×K	691.81	Joback Method
cps	165.20	J/mol×K	298.15	NIST Webbook
cps	124.30	J/mol×K	293.00	NIST Webbook
hfust	17.19	kJ/mol	317.00	NIST Webbook
hfust	17.30	kJ/mol	316.55	NIST Webbook
hfust	17.89	kJ/mol	316.50	NIST Webbook
hfust	17.89	kJ/mol	316.50	NIST Webbook
hfust	17.30	kJ/mol	316.60	NIST Webbook
hfust	18.90	kJ/mol	316.90	NIST Webbook
hfust	17.28	kJ/mol	315.60	NIST Webbook
hfust	17.28	kJ/mol	315.60	NIST Webbook
hvapt	51.10	kJ/mol	433.50	NIST Webbook
hvapt	54.90	kJ/mol	394.00	NIST Webbook
rhol	964.00	kg/m3	323.00	KDB
sfust	55.00	J/mol×K	316.55	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.47492e+01
Coeff. B	-4.06450e+03
Coeff. C	-7.28020e+01
Temperature range (K), min.	316.90
Temperature range (K), max.	503.47

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	7.87351e+01
Coeff. B	-9.11716e+03
Coeff. C	-9.05134e+00
Coeff. D	3.95560e-06
Temperature range (K), min.	316.90
Temperature range (K), max.	693.15

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C106490&Units=SI
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
KDB Vapor Pressure Data:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1299
Estimated Solubility Method:	http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
KDB:	https://www.cheric.org/files/research/kdb/mol/mol1299.mol
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

af:	Acentric Factor
affp:	Proton affinity
basg:	Gas basicity
chl:	Standard liquid enthalpy of combustion
cpg:	Ideal gas heat capacity
cps:	Solid phase heat capacity
dm:	Dipole Moment
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfl:	Liquid 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
hvap:	Enthalpy of vaporization at standard conditions
hvapt:	Enthalpy of vaporization at a given temperature
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
pvap:	Vapor pressure
rhol:	Liquid Density
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
sfust:	Entropy of fusion at a given temperature
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume