1,3-Phenylenediamine

Other names: 1,3-BENZENEDIAMINE
1,3-Diaminobenzene
3-Aminoaniline
APCO 2330
C.I. 76025
C.I. Developer 11
Developer 11
Developer C
Developer H
Developer M
Direct Brown BR
Direct Brown GG
M-BENZENEDIAMINE
Metaphenylenediamine
NSC 4776
Phenylenediamine, m
Phenylenediamine, meta
UN-1673
m-Aminoaniline
m-Diaminobenzene
m-Fenylendiamin
m-Phenylenediamine

Inchi: InChI=1S/C6H8N2/c7-5-2-1-3-6(8)4-5/h1-4H,7-8H2
InchiKey: WZCQRUWWHSTZEM-UHFFFAOYSA-N
Formula: C6H8N2
SMILES: Nc1cccc(N)c1
Mol. weight [g/mol]: 108.14
CAS: 108-45-2

Physical Properties

Property code	Value	Unit	Source
af	0.5580		KDB
affp	929.90	kJ/mol	NIST Webbook
basg	899.20	kJ/mol	NIST Webbook
chs	-3497.00 ± 5.40	kJ/mol	NIST Webbook
gf	235.32	kJ/mol	Joback Method

hf	125.47	kJ/mol	Joback Method
hfs	-7.90	kJ/mol	NIST Webbook
hfus	15.34	kJ/mol	Joback Method
hsub	90.40 ± 0.40	kJ/mol	NIST Webbook
hvap	53.17	kJ/mol	Joback Method
ie	7.60	eV	NIST Webbook
ie	7.50 ± 0.10	eV	NIST Webbook
ie	7.96	eV	NIST Webbook
ie	7.74	eV	NIST Webbook
ie	7.14	eV	NIST Webbook
ie	7.44	eV	NIST Webbook
log10ws	-0.74		Crippen Method
logp	0.851		Crippen Method
mcvol	91.600	ml/mol	McGowan Method
pc	4800.00	kPa	KDB
rinpol	1303.00		NIST Webbook
ss	149.49	J/mol×K	NIST Webbook
ss	154.50	J/mol×K	NIST Webbook
tb	556.20	K	NIST Webbook
tb	558.20	K	KDB
tc	815.00	K	KDB
tf	337.00	K	NIST Webbook
tf	336.00	K	KDB
tf	335.00 ± 0.40	K	NIST Webbook
tt	339.10 ± 0.50	K	NIST Webbook
vc	0.322	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	247.46	J/mol×K	757.17	Joback Method
cpg	240.43	J/mol×K	716.54	Joback Method
cpg	232.82	J/mol×K	675.91	Joback Method
cpg	224.60	J/mol×K	635.29	Joback Method
cpg	215.73	J/mol×K	594.66	Joback Method
cpg	206.18	J/mol×K	554.03	Joback Method
cpg	195.92	J/mol×K	513.40	Joback Method
cpl	153.70	J/mol×K	298.00	NIST Webbook
cps	161.08	J/mol×K	300.00	NIST Webbook
cps	159.60	J/mol×K	298.15	NIST Webbook
hfust	15.40	kJ/mol	335.50	NIST Webbook

hfust	15.40	kJ/mol	335.50	NIST Webbook
hfust	15.57	kJ/mol	339.10	NIST Webbook
hvapt	63.70	kJ/mol	465.50	NIST Webbook
sfust	45.92	J/mol×K	339.10	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.65536e+01
Coeff. B	-6.10312e+03
Coeff. C	-4.48490e+01
Temperature range (K), min.	420.06
Temperature range (K), max.	587.73

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	6.10587e+01
Coeff. B	-9.88864e+03
Coeff. C	-6.21494e+00
Coeff. D	1.78547e-06
Temperature range (K), min.	334.00
Temperature range (K), max.	824.00

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
KDB:	https://www.cheric.org/files/research/kdb/mol/mol1294.mol
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C108452&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
KDB Vapor Pressure Data:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1294
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

af:	Acentric Factor
affp:	Proton affinity
basg:	Gas basicity
chs:	Standard solid enthalpy of combustion
cpg:	Ideal gas heat capacity
cpl:	Liquid phase heat capacity
cps:	Solid phase 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
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
rinpol:	Non-polar retention indices
sfust:	Entropy of fusion at a given temperature
ss:	Solid phase molar entropy at standard conditions
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
tt:	Triple Point Temperature
vc:	Critical Volume

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