2-Naphthalenamine

Other names:	2-AMINONAPHTHALENE
	2-Aminonaftalen
	2-Naftylamin
	2-Naftylamine
	2-Naphthalamine
	2-Naphthylamin
	2-Naphthylamine
	6-Naphthylamine
	BETA-NAPHTHYLAMINE
	C.I. 37270
	Fast Scarlet Base B
	RCRA waste number U168
	UN 1650
	USAF CB-22
	«beta»-Naftalamin
	«beta»-Naftilamina
	«beta»-Naftylamin
	«beta»-Naphthylamin
	«beta»-Naphthylamine
	«beta»-naftyloamina
	Â«betaÂ»-Naftalamin
	Â«betaÂ»-Naftilamina
	Â«betaÂ»-Naftylamin
	Â«betaÂ»-Naphthylamin
	Â«betaÂ»-Naphthylamine
	Â«betaÂ»-naftyloamina
Inchi:	InChI=1S/C10H9N/c11-10-6-5-8-3-1-2-4-9(8)7-10/h1-7H,11H2
InchiKey:	JBIJLHTVPXGSAM-UHFFFAOYSA-N
Formula:	C10H9N
SMILES:	Nc1ccc2ccccc2c1
Mol. weight [g/mol]:	143.19
CAS:	91-59-8

Physical Properties

Property code	Value	Unit	Source
chs	-5303.20	kJ/mol	NIST Webbook

chs	-5304.10	kJ/mol	NIST Webbook
chs	-5279.00 ± 4.60	kJ/mol	NIST Webbook
chs	-5301.00	kJ/mol	NIST Webbook
chs	-5284.00 ± 5.40	kJ/mol	NIST Webbook
gf	309.20	kJ/mol	Joback Method
hf	200.19	kJ/mol	Joback Method
hfs	81.60	kJ/mol	NIST Webbook
hfs	79.90	kJ/mol	NIST Webbook
hfs	77.80	kJ/mol	NIST Webbook
hfus	17.52	kJ/mol	Joback Method
hsub	73.90	kJ/mol	NIST Webbook
hvap	53.07	kJ/mol	Joback Method
ie	7.10 ± 0.10	eV	NIST Webbook
ie	7.56	eV	NIST Webbook
ie	7.03	eV	NIST Webbook
ie	7.10 ± 0.02	eV	NIST Webbook
ie	7.40 ± 0.10	eV	NIST Webbook
ie	7.55	eV	NIST Webbook
ie	7.50	eV	NIST Webbook
ie	7.20	eV	NIST Webbook
log10ws	-2.91		Crippen Method
logp	2.422		Crippen Method
mcvol	118.520	ml/mol	McGowan Method
pc	4109.14	kPa	Joback Method
rinpol	1486.00		NIST Webbook
rinpol	264.85		NIST Webbook
rinpol	265.53		NIST Webbook
rinpol	1486.00		NIST Webbook
rinpol	264.34		NIST Webbook
rinpol	264.62		NIST Webbook
rinpol	1484.80		NIST Webbook
rinpol	1535.00		NIST Webbook
rinpol	1562.00		NIST Webbook
rinpol	1510.20		NIST Webbook
rinpol	264.23		NIST Webbook
tb	579.20	K	NIST Webbook
tc	800.58	K	Joback Method
tf	385.15 ± 1.00	K	NIST Webbook
tf	383.30 ± 0.25	K	NIST Webbook
tf	383.15 ± 0.40	K	NIST Webbook
tf	383.15 ± 2.00	K	NIST Webbook
tf	381.15 ± 2.00	K	NIST Webbook
tf	386.15 ± 1.50	K	NIST Webbook
tf	382.70 ± 0.20	K	NIST Webbook

tf	383.00 ± 5.00	K	NIST Webbook
vc	0.439	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	275.40	J/mol×K	592.90	Joback Method
cpg	287.23	J/mol×K	634.44	Joback Method
cpg	298.07	J/mol×K	675.97	Joback Method
cpg	308.03	J/mol×K	717.51	Joback Method
cpg	317.19	J/mol×K	759.04	Joback Method
cpg	262.52	J/mol×K	551.37	Joback Method
cpg	325.62	J/mol×K	800.58	Joback Method
cps	125.90	J/mol×K	293.00	NIST Webbook
hfust	23.33	kJ/mol	386.20	NIST Webbook
hfust	23.33	kJ/mol	386.20	NIST Webbook
hsubt	74.06 ± 0.84	kJ/mol	283.00	NIST Webbook
hvapt	63.50	kJ/mol	483.50	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.58954e+01
Coeff. B	-6.02170e+03
Coeff. C	-4.52210e+01
Temperature range (K), min.	424.05
Temperature range (K), max.	614.17

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	6.77806e+01
Coeff. B	-1.02120e+04
Coeff. C	-7.30827e+00
Coeff. D	2.86143e-06

Temperature range (K), min.	388.15
Temperature range (K), max.	579.15

Sources

KDB Vapor Pressure Data:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1310
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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/mol1310.mol
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C91598&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

Legend

chs:	Standard solid enthalpy of combustion
cpg:	Ideal gas 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
hsubt:	Enthalpy of sublimation at a given temperature
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point

vc: Critical Volume