1-Naphthalenamine

Other names:	.alpha.-aminonaphthalene
	.alpha.-naphthylamine
	1-AMINONAPHTHALENE
	1-Aminonaftalen
	1-Naftilamina
	1-Naftylamin
	1-Naftylamine
	1-Naphthalamine
	1-Naphthylamin
	1-Naphthylamine
	1-Napthylamine
	ALPHA-AMINONAPHTHALENE
	Alfa-naftyloamina
	Alfanaftilamina
	C.I. 37265
	C.I. Azoic Diazo Component 114
	Fast Garnet Base B
	Fast garnet B base
	Naphthalen-1-ylamine
	Naphthalidam
	Naphthalidine
	Rcra waste number U167
	UN 2077
	«alpha»-Aminonaphthalene
	«alpha»-Naftalamin
	«alpha»-Naftylamin
	«alpha»-Naphthylamine
	Â«alphaÂ»-Aminonaphthalene
	Â«alphaÂ»-Naftalamin
	Â«alphaÂ»-Naftylamin
	Â«alphaÂ»-Naphthylamine
Inchi:	InChI=1S/C10H9N/c11-10-7-3-5-8-4-1-2-6-9(8)10/h1-7H,11H2
InchiKey:	RUFPHBVGCFYCNW-UHFFFAOYSA-N
Formula:	C10H9N
SMILES:	Nc1cccc2ccccc12
Mol. weight [g/mol]:	143.19
CAS:	134-32-7

Physical Properties

Property code	Value	Unit	Source
affp	907.00	kJ/mol	NIST Webbook
basg	875.10	kJ/mol	NIST Webbook
chs	-5285.90 ± 5.30	kJ/mol	NIST Webbook
chs	-5312.80	kJ/mol	NIST Webbook
chs	-5289.00 ± 5.40	kJ/mol	NIST Webbook
chs	-5314.00	kJ/mol	NIST Webbook
chs	-5308.49	kJ/mol	NIST Webbook
gf	309.20	kJ/mol	Joback Method
hf	200.19	kJ/mol	Joback Method
hfs	92.50	kJ/mol	NIST Webbook
hfs	91.60	kJ/mol	NIST Webbook
hfs	87.00	kJ/mol	NIST Webbook
hfus	17.52	kJ/mol	Joback Method
hsub	88.10 ± 0.40	kJ/mol	NIST Webbook
hvap	73.30 ± 0.40	kJ/mol	NIST Webbook
ie	7.40	eV	NIST Webbook
ie	7.39	eV	NIST Webbook
ie	7.30	eV	NIST Webbook
ie	7.48	eV	NIST Webbook
ie	7.30 ± 0.10	eV	NIST Webbook
ie	7.09	eV	NIST Webbook
ie	7.46	eV	NIST Webbook
log10ws	-1.92		Aqueous Solubility Prediction Method
log10ws	-1.92		Estimated Solubility Method
logp	2.422		Crippen Method
mcvol	118.520	ml/mol	McGowan Method
pc	4109.14	kPa	Joback Method
rinpol	262.17		NIST Webbook
rinpol	1515.70		NIST Webbook
rinpol	1495.10		NIST Webbook
rinpol	1531.00		NIST Webbook
rinpol	1531.00		NIST Webbook
rinpol	262.17		NIST Webbook
rinpol	1495.10		NIST Webbook
rinpol	262.98		NIST Webbook
rinpol	262.55		NIST Webbook
rinpol	1531.00		NIST Webbook

rinpol	1515.70		NIST Webbook
rinpol	1550.00		NIST Webbook
rinpol	261.01		NIST Webbook
rinpol	262.20		NIST Webbook
tb	512.10 ± 27.77	K	NIST Webbook
tb	574.00	K	NIST Webbook
tb	573.15 ± 2.00	K	NIST Webbook
tb	573.95 ± 1.50	K	NIST Webbook
tc	800.58	K	Joback Method
tf	323.00	K	Vapor Pressures and Phase Transitions of a Series of the Aminonaphthalenes
tf	321.88	K	Aqueous Solubility Prediction Method
vc	0.439	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	262.52	J/mol×K	551.37	Joback Method
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	325.62	J/mol×K	800.58	Joback Method
hfust	15.53	kJ/mol	323.20	NIST Webbook
hfust	15.53	kJ/mol	323.20	NIST Webbook
hvapt	63.60	kJ/mol	475.50	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.60427e+01
Coeff. B	-6.10996e+03
Coeff. C	-3.91810e+01

Temperature range (K), min.	426.99
Temperature range (K), max.	608.54

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	7.09079e+01
Coeff. B	-1.03031e+04
Coeff. C	-7.77314e+00
Coeff. D	3.16272e-06
Temperature range (K), min.	377.15
Temperature range (K), max.	574.15

Sources

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

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=1309

Densities and Viscosities of Naphthalen-1-ol, Naphthalen-2-ol, and 1-Aminonaphthalene in the Solvents of Ethanol, Propan-1-ol, and Butan-1-ol: https://www.doi.org/10.1021/je201222n

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

KDB: https://www.cheric.org/files/research/kdb/mol/mol1309.mol

Estimated Solubility Method: http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C134327&Units=SI

Vapor Pressures and Phase Transitions of a Series of the Aminonaphthalenes: https://www.doi.org/10.1021/je060394v

Aqueous Solubility Prediction Method: http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

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
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