1-Naphthalenamine, N-phenyl-

Other names:	1-Naphthylamine, N-phenyl-
	«alpha»-Naphthylphenylamine
	Antioxidant PAN
	C.I. 44050
	N-(1-Naphthyl)aniline
	N-Phenyl-«alpha»-naphthylamine
	N-Phenyl-1-naphthylamine
	Neozone A
	Nonox A
	Phenyl-«alpha»-naphthylamine
	Phenyl-1-naphthylamine
	«alpha»-Phenylnaphthylamine
	Aceto PAN
	Phenylnaphthylamine
	1-Anilinonaphthalene
	Additin 30
	N-Fenyl-1-aminonaftalen
	Fenyl-«alpha»-naftylamin
	Neozon A
	PANA
	Vulkanox PAN
	Nonox AN
	N-Phenyl-1-naphthalenamine
	N-Phenyl-1-aminonaphthalene
	Nocrac PA
	Algerite
	Naugard PANA
	1-Naphthyl phenyl amine
	Amoco 32
	NSC 2622
Inchi:	InChI=1S/C16H13N/c1-2-9-14(10-3-1)17-16-12-6-8-13-7-4-5-11-15(13)16/h1-12,17H
InchiKey:	XQVWYOYUZDUNRW-UHFFFAOYSA-N
Formula:	C16H13N
SMILES:	c1ccc(Nc2cccc3ccccc23)cc1
Mol. weight [g/mol]:	219.28
CAS:	90-30-2

Physical Properties

Property code	Value	Unit	Source
chs	-8447.50	kJ/mol	NIST Webbook
gf	495.07	kJ/mol	Joback Method
hf	332.56	kJ/mol	Joback Method
hfs	293.00	kJ/mol	NIST Webbook
hfus	27.01	kJ/mol	Joback Method
hvap	64.50	kJ/mol	Joback Method
ie	7.12	eV	NIST Webbook
log10ws	-5.08		Crippen Method
logp	4.583		Crippen Method
mcvol	179.300	ml/mol	McGowan Method
pc	2925.00	kPa	Joback Method
rinpol	2135.00		NIST Webbook
rinpol	2135.00		NIST Webbook
rinpol	2135.00		NIST Webbook
tb	692.97	K	Joback Method
tc	951.41	K	Joback Method
tf	332.15	K	NIST Webbook
vc	0.672	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	518.61	J/mol×K	865.26	Joback Method
cpg	529.70	J/mol×K	908.34	Joback Method
cpg	463.28	J/mol×K	692.97	Joback Method
cpg	479.04	J/mol×K	736.04	Joback Method
cpg	493.42	J/mol×K	779.12	Joback Method
cpg	506.56	J/mol×K	822.19	Joback Method
cpg	539.99	J/mol×K	951.41	Joback Method
hsubt	96.50	kJ/mol	323.00	NIST Webbook
hvapt	89.60	kJ/mol	353.00	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	499.20	K	2.00	NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C90302&Units=SI
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

Legend

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
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
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