N-Nitrosodiphenylamine

Other names:	Benzenamine, N-nitroso-N-phenyl-
	Curetard A
	Delac J
	Difenylnitrosamin
	Diphenyl N-nitrosoamine
	Diphenylamine, N-nitroso-
	Diphenylnitrosamin
	Diphenylnitrosamine
	N,N-Diphenyl-N-nitrosoamine
	N,N-Diphenylnitrosamine
	N-Nitroso-N-diphenylamine
	N-Nitroso-N-phenylaniline
	N-Nitrosodifenylamin
	N-nitroso-N-phenylbenzenamine
	NCI-C02880
	NSC 585
	Naugard tjb
	Ndpa
	NdphA
	Nitrosodiphenylamine
	Ortard
	Redax
	Retarder J
	Sconoc
	TJB
	Vulcalent A
	Vulcatard
	Vulcatard A
	Vulkalent A
	Vultrol
	diphenylamine, N-nitroso
Inchi:	InChI=1S/C12H10N2O/c15-13-14(11-7-3-1-4-8-11)12-9-5-2-6-10-12/h1-10H
InchiKey:	UBUCNCOMADRQHX-UHFFFAOYSA-N
Formula:	C12H10N2O
SMILES:	O=NN(c1ccccc1)c1ccccc1
Mol. weight [g/mol]:	198.22
CAS:	86-30-6

Physical Properties

Property code	Value	Unit	Source
chs	-6378.50 ± 6.30	kJ/mol	NIST Webbook
chs	-6388.59	kJ/mol	NIST Webbook
hf	81.39	kJ/mol	Joback Method
hfs	227.00 ± 6.30	kJ/mol	NIST Webbook
hfs	237.30	kJ/mol	NIST Webbook
hfus	11.06	kJ/mol	Measurement and prediction of (solid + liquid) equilibria of gun powder's and propellant's stabilizers mixtures
hvap	58.00	kJ/mol	Joback Method
log10ws	-3.75		Aqueous Solubility Prediction Method
logp	3.506		Crippen Method
mcvol	153.950	ml/mol	McGowan Method
pc	3348.98	kPa	Joback Method
rinpol	274.90		NIST Webbook
rinpol	1865.00		NIST Webbook
tb	603.16	K	Joback Method
tc	840.69	K	Joback Method
tf	339.65	K	Aqueous Solubility Prediction Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C86306&Units=SI

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

Measurement and prediction of (solid + liquid) equilibria of gun powder's and propellant's stabilizers mixtures: https://www.doi.org/10.1016/j.jct.2010.03.025

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

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

chs: Standard solid enthalpy of combustion

hf:	Enthalpy of formation at standard conditions
hfs:	Solid phase enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
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
tc:	Critical Temperature
tf:	Normal melting (fusion) point