Benzenamine, 2-nitro-N-phenyl-

Other names:	2-Nitro-N-phenylaniline 2-nitrodiphenylamine C.I. 10335 Diphenylamine, 2-nitro- N-Phenyl-2-nitrobenzenamine N-Phenyl-o-Nitroaniline NSC 105613 Sudan Yellow 1339 benzeneamine, 2-nitro-N-phenyl- o-(Phenylamino)nitrobenzene o-Nitro-N-phenylaniline o-Nitrodiphenylamine phenyl-2-nitrophenylamine
Inchi:	InChI=1S/C12H10N2O2/c15-14(16)12-9-5-4-8-11(12)13-10-6-2-1-3-7-10/h1-9,13H
InchiKey:	RUKISNQKOIKZGT-UHFFFAOYSA-N
Formula:	C12H10N2O2
SMILES:	O=[N+]([O-])c1ccccc1Nc1ccccc1
Mol. weight [g/mol]:	214.22
CAS:	119-75-5

Physical Properties

Property code	Value	Unit	Source
chs	-6215.80 ± 6.30	kJ/mol	NIST Webbook
chs	-6228.00 ± 2.00	kJ/mol	NIST Webbook
gf	390.29	kJ/mol	Joback Method
hf	213.29	kJ/mol	Joback Method
hfs	64.50 ± 6.30	kJ/mol	NIST Webbook
hfs	77.00 ± 2.00	kJ/mol	NIST Webbook
hfus	26.14	kJ/mol	Measurement and prediction of (solid + liquid) equilibria of gun powder's and propellant's stabilizers mixtures
hvap	70.55	kJ/mol	Joback Method
log10ws	-3.93		Crippen Method
logp	3.338		Crippen Method
mcvol	159.820	ml/mol	McGowan Method
pc	3468.36	kPa	Joback Method

rinpol	335.70		NIST Webbook
rinpol	1886.00		NIST Webbook
tb	734.31	K	Joback Method
tc	1004.26	K	Joback Method
tf	347.90	K	Experimental and modeling studies of binary organic eutectic systems to be used as stabilizers for nitrate esters-based energetic materials
tf	348.10 ± 0.15	K	NIST Webbook
tf	348.10 ± 0.20	K	NIST Webbook
tf	347.90 ± 0.30	K	NIST Webbook
vc	0.609	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	421.30	J/mol×K	734.31	Joback Method
cpg	434.25	J/mol×K	779.30	Joback Method
cpg	445.95	J/mol×K	824.29	Joback Method
cpg	456.48	J/mol×K	869.29	Joback Method
cpg	465.95	J/mol×K	914.28	Joback Method
cpg	474.47	J/mol×K	959.27	Joback Method
cpg	482.14	J/mol×K	1004.26	Joback Method
hsubt	100.90	kJ/mol	340.50	NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Experimental and modeling studies of binary organic eutectic systems to be used as stabilizers for nitrate esters-based energetic materials:	https://www.doi.org/10.1016/j.fluid.2019.06.021
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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C119755&Units=SI

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
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
vc:	Critical Volume