Hydrazine, phenyl-

Other names:	1-Phenylhydrazine
	Fenilidrazina
	Fenylhydrazine
	HYDRAZINOBENZENE
	Monophenylhydrazine
	Phenylhydrazin
	Phenylhydrazine
	UN 2572
	phenyl hydrazine
Inchi:	InChI=1S/C6H8N2/c7-8-6-4-2-1-3-5-6/h1-5,8H,7H2
InchiKey:	HKOOXMFOFWEVGF-UHFFFAOYSA-N
Formula:	C6H8N2
SMILES:	NNc1ccccc1
Mol. weight [g/mol]:	108.14
CAS:	100-63-0

Physical Properties

Property code	Value	Unit	Source
chl	-3647.00 ± 3.00	kJ/mol	NIST Webbook
chl	-3683.60	kJ/mol	NIST Webbook
chl	-3645.40 ± 0.84	kJ/mol	NIST Webbook
chl	-3646.60	kJ/mol	NIST Webbook
gf	267.89	kJ/mol	Joback Method
hf	204.10	kJ/mol	NIST Webbook
hf	202.90 ± 1.20	kJ/mol	NIST Webbook
hf	205.00 ± 13.00	kJ/mol	NIST Webbook
hf	240.90	kJ/mol	NIST Webbook
hfl	142.20	kJ/mol	NIST Webbook
hfl	141.00 ± 0.80	kJ/mol	NIST Webbook
hfl	179.00	kJ/mol	NIST Webbook
hfus	15.63	kJ/mol	Joback Method
hvap	61.90 ± 0.80	kJ/mol	NIST Webbook
hvap	61.90	kJ/mol	NIST Webbook
hvap	61.46	kJ/mol	NIST Webbook
ie	7.86	eV	NIST Webbook
ie	7.64 ± 0.02	eV	NIST Webbook
ie	7.74	eV	NIST Webbook

log10ws	0.07		Estimated Solubility Method
log10ws	0.07		Aqueous Solubility Prediction Method
logp	0.972		Crippen Method
mcvol	91.600	ml/mol	McGowan Method
nfpaf	%!d(float64=2)		KDB
nfpah	%!d(float64=3)		KDB
pc	5153.45	kPa	Joback Method
rinpol	1157.00		NIST Webbook
tb	516.65 ± 1.00	K	NIST Webbook
tb	516.20	K	NIST Webbook
tb	512.70	K	NIST Webbook
tc	717.56	K	Joback Method
tf	292.15	K	KDB
tf	292.45	K	Aqueous Solubility Prediction Method
tf	292.80 ± 0.02	K	NIST Webbook
tf	283.15 ± 1.50	K	NIST Webbook
tf	295.00 ± 0.50	K	NIST Webbook
vc	0.328	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	188.20	J/mol×K	486.06	Joback Method
cpg	235.86	J/mol×K	678.98	Joback Method
cpg	227.71	J/mol×K	640.39	Joback Method
cpg	218.91	J/mol×K	601.81	Joback Method
cpg	209.41	J/mol×K	563.23	Joback Method
cpg	199.19	J/mol×K	524.64	Joback Method
cpg	243.39	J/mol×K	717.56	Joback Method
cpl	217.30	J/mol×K	299.45	NIST Webbook
hfust	16.43	kJ/mol	292.80	NIST Webbook
hfust	16.43	kJ/mol	292.80	NIST Webbook
hvapt	57.20	kJ/mol	421.50	NIST Webbook
hvapt	59.20	kJ/mol	431.00	NIST Webbook
hvapt	57.30	kJ/mol	465.50	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.60520e+01
Coeff. B	-5.13721e+03
Coeff. C	-6.33960e+01
Temperature range (K), min.	389.27
Temperature range (K), max.	541.70

Sources

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

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

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C100630&Units=SI

The Yaws Handbook of Vapor Pressure: https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

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

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

KDB: https://www.cheric.org/files/research/kdb/mol/mol1470.mol

Legend

chl: Standard liquid enthalpy of combustion

cpg: Ideal gas heat capacity

cpl: Liquid phase heat capacity

gf: Standard Gibbs free energy of formation

hf: Enthalpy of formation at standard conditions

hfl: Liquid phase enthalpy of formation at standard conditions

hfus: Enthalpy of fusion at standard conditions

hfust: Enthalpy of fusion 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
nfpaf:	NFPA Fire Rating
nfpah:	NFPA Health Rating
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