Phenol, 4-nitro-

Other names:	1-Hydroxy-4-nitrobenzene
	4-Hydroxynitrobenzene
	4-Nitrofenol
	4-Nitrophenol
	4-hydroxy-1-nitrobenzene
	NCI-C55992
	NSC 1317
	Niphen
	PNP
	Paranitrofenol
	Paranitrofenolo
	Paranitrophenol
	Phenol, p-nitro-
	Rcra waste number U170
	p-Hydroxynitrobenzene
	p-Nitrofenol
	p-Nitrophenol
Inchi:	InChI=1S/C6H5NO3/c8-6-3-1-5(2-4-6)7(9)10/h1-4,8H
InchiKey:	BTJIUGUIPKRLHP-UHFFFAOYSA-N
Formula:	C6H5NO3
SMILES:	O=[N+]([O-])c1ccc(O)cc1
Mol. weight [g/mol]:	139.11
CAS:	100-02-7

Physical Properties

Property code	Value	Unit	Source
chs	-2863.21 ± 0.54	kJ/mol	NIST Webbook
chs	-2874.00	kJ/mol	NIST Webbook
chs	-2879.60	kJ/mol	NIST Webbook
chs	-2868.50 ± 1.00	kJ/mol	NIST Webbook
chs	-2848.90	kJ/mol	NIST Webbook
gf	-7.02	kJ/mol	Joback Method
hf	-114.70 ± 1.20	kJ/mol	NIST Webbook
hf	-117.70 ± 2.00	kJ/mol	NIST Webbook
hfs	-207.10 ± 1.10	kJ/mol	NIST Webbook
hfs	-226.70	kJ/mol	NIST Webbook
hfs	-209.00	kJ/mol	NIST Webbook

hfs	-212.40 ± 1.00	kJ/mol	NIST Webbook
hfus	22.48	kJ/mol	Joback Method
hsub	99.00 ± 1.00	kJ/mol	NIST Webbook
hsub	92.40	kJ/mol	NIST Webbook
hsub	92.39 ± 0.43	kJ/mol	NIST Webbook
hvap	60.83	kJ/mol	Joback Method
ie	7.38	eV	NIST Webbook
ie	9.10	eV	NIST Webbook
ie	9.38	eV	NIST Webbook
ie	9.52	eV	NIST Webbook
ie	8.80 ± 0.10	eV	NIST Webbook
log10ws	-0.74		Aqueous Solubility Prediction Method
log10ws	-0.74		Estimated Solubility Method
logp	1.300		Crippen Method
mcvol	94.930	ml/mol	McGowan Method
pc	5899.00	kPa	Joback Method
rinpol	1588.00		NIST Webbook
rinpol	1530.00		NIST Webbook
rinpol	1546.00		NIST Webbook
rinpol	260.40		NIST Webbook
rinpol	1546.00		NIST Webbook
rinpol	1546.10		NIST Webbook
rinpol	1530.00		NIST Webbook
rinpol	1539.00		NIST Webbook
rinpol	1527.20		NIST Webbook
rinpol	1544.80		NIST Webbook
rinpol	1562.00		NIST Webbook
rinpol	1546.10		NIST Webbook
rinpol	262.33		NIST Webbook
tb	552.20	K	NIST Webbook
tc	861.12	K	Joback Method
tf	386.95	K	KDB
tf	386.41	K	Aqueous Solubility Prediction Method
vc	0.311	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	261.56	J/mol×K	861.12	Joback Method

cpg	235.93	J/mol×K	684.25	Joback Method
cpg	243.08	J/mol×K	728.47	Joback Method
cpg	249.65	J/mol×K	772.69	Joback Method
cpg	255.77	J/mol×K	816.90	Joback Method
cpg	228.08	J/mol×K	640.04	Joback Method
cpg	219.41	J/mol×K	595.82	Joback Method
cps	144.00	J/mol×K	283.00	NIST Webbook
hfust	24.27	kJ/mol	387.00	NIST Webbook
hfust	18.25	kJ/mol	388.20	NIST Webbook
hfust	18.25	kJ/mol	388.20	NIST Webbook
hfust	11.00	kJ/mol	386.40	NIST Webbook
hfust	18.25	kJ/mol	387.00	NIST Webbook
hfust	19.30	kJ/mol	368.75	NIST Webbook
hfust	30.12	kJ/mol	385.15	NIST Webbook
hsubt	91.20 ± 1.70	kJ/mol	345.00	NIST Webbook
hsubt	91.00 ± 2.00	kJ/mol	343.00	NIST Webbook
sfust	62.70	J/mol×K	387.00	NIST Webbook
sfust	52.30	J/mol×K	368.75	NIST Webbook
sfust	78.20	J/mol×K	385.15	NIST Webbook
sfust	47.17	J/mol×K	387.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	9.12213e+00
Coeff. B	-2.13960e+03
Coeff. C	-7.71340e+01
Temperature range (K), min.	319.32
Temperature range (K), max.	638.61

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	7.50049e+01
Coeff. B	-1.28318e+04
Coeff. C	-7.64739e+00
Coeff. D	3.52466e-06
Temperature range (K), min.	415.15

Temperature range (K), max.	459.15

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C100027&Units=SI
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
Thermodynamic properties of paracetamol impurities 4-nitrophenol and 4-chloroacetanilide and the impact of such impurities on the crystallisation of paracetamol from solution:	https://www.doi.org/10.1016/j.jct.2019.02.004
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Enhanced partition model of 4-nitrophenol in water - octanol system.	https://www.doi.org/10.1016/j.fluid.2016.08.021
Estimated Solubility Method:	http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt
Effects of association/dissociation processes:	
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
KDB Vapor Pressure Data:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1442
KDB:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1442

Legend

chs:	Standard solid enthalpy of combustion
cpg:	Ideal gas heat capacity
cps:	Solid phase 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
hsubt:	Enthalpy of sublimation at a given temperature
hvap:	Enthalpy of vaporization at standard conditions
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
sfust:	Entropy of fusion at a given temperature
tb:	Normal Boiling Point Temperature

tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume