Phenol, 2-nitro-

Other names:	2-Hydroxynitrobenzene
	2-Nitrophenol
	Phenol, o-nitro-
	UN 1663
	o-Hydroxynitrobenzene
	o-Nitrofenol
	o-Nitrophenol
Inchi:	InChI=1S/C6H5NO3/c8-6-4-2-1-3-5(6)7(9)10/h1-4,8H
InchiKey:	IQUPABOKLQSFBK-UHFFFAOYSA-N
Formula:	C6H5NO3
SMILES:	O=[N+]([O-])c1ccccc1O
Mol. weight [g/mol]:	139.11
CAS:	88-75-5

Physical Properties

Property code	Value	Unit	Source
chs	-2878.80	kJ/mol	NIST Webbook
chs	-2871.00 ± 1.30	kJ/mol	NIST Webbook
chs	-2873.27 ± 0.62	kJ/mol	NIST Webbook
chs	-2876.30	kJ/mol	NIST Webbook
chs	-2887.00	kJ/mol	NIST Webbook
gf	-7.02	kJ/mol	Joback Method
hf	-132.30 ± 1.40	kJ/mol	NIST Webbook
hf	-128.80 ± 1.60	kJ/mol	NIST Webbook
hfs	-204.60 ± 1.40	kJ/mol	NIST Webbook
hfs	-210.00	kJ/mol	NIST Webbook
hfs	-199.30	kJ/mol	NIST Webbook
hfs	-202.40 ± 1.00	kJ/mol	NIST Webbook
hfus	22.48	kJ/mol	Joback Method
hsub	72.30 ± 0.28	kJ/mol	NIST Webbook
hsub	73.30	kJ/mol	NIST Webbook
hvap	58.40 ± 0.50	kJ/mol	NIST Webbook
ie	9.29	eV	NIST Webbook
ie	9.10	eV	NIST Webbook
log10ws	-1.74		Aqueous Solubility Prediction Method

log10ws	-1.74		Estimated Solubility Method
logp	1.300		Crippen Method
mcvol	94.930	ml/mol	McGowan Method
pc	5899.00	kPa	Joback Method
rinpol	1127.00		NIST Webbook
rinpol	1126.00		NIST Webbook
rinpol	1149.00		NIST Webbook
rinpol	1154.10		NIST Webbook
rinpol	1133.00		NIST Webbook
rinpol	1099.00		NIST Webbook
rinpol	188.90		NIST Webbook
rinpol	1166.00		NIST Webbook
rinpol	1149.00		NIST Webbook
rinpol	1136.00		NIST Webbook
rinpol	189.22		NIST Webbook
ripol	1818.00		NIST Webbook
ripol	1812.00		NIST Webbook
ripol	1814.00		NIST Webbook
ripol	1818.00		NIST Webbook
tb	490.40 ± 0.40	K	NIST Webbook
tb	490.35	K	KDB
tb	489.20	K	NIST Webbook
tb	490.40 ± 0.70	K	NIST Webbook
tc	861.12	K	Joback Method
tf	317.91	K	Aqueous Solubility Prediction Method
tf	318.05	K	KDB
vc	0.311	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	255.77	J/mol×K	816.90	Joback Method
cpg	219.41	J/mol×K	595.82	Joback Method
cpg	228.08	J/mol×K	640.04	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	261.56	J/mol×K	861.12	Joback Method
hfust	17.45	kJ/mol	318.20	NIST Webbook
hfust	17.45	kJ/mol	318.00	NIST Webbook

hfust	17.05	kJ/mol	316.30	NIST Webbook
hfust	17.45	kJ/mol	318.20	NIST Webbook
hsubt	73.20 ± 1.30	kJ/mol	304.00	NIST Webbook
hsubt	54.80	kJ/mol	282.50	NIST Webbook
hsubt	73.00 ± 2.00	kJ/mol	303.00	NIST Webbook
hvapt	54.40	kJ/mol	339.50	NIST Webbook
hvapt	55.90	kJ/mol	428.00	NIST Webbook
sfust	54.86	J/mol×K	318.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.07924e+01
Coeff. B	-2.54411e+03
Coeff. C	-7.71340e+01
Temperature range (K), min.	319.32
Temperature range (K), max.	541.31

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	1.39908e+02
Coeff. B	-1.23899e+04
Coeff. C	-1.81502e+01
Coeff. D	9.65481e-06
Temperature range (K), min.	364.15
Temperature range (K), max.	495.15

Sources

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

KDB: https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1443

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C88755&Units=SI

KDB Vapor Pressure Data: https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1443

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Estimated Solubility Method:	http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

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
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
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
pvap:	Vapor pressure
rinpol:	Non-polar retention indices
ripol:	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