

Phenol, 3-nitro-

Other names:	1-Hydroxy-3-nitrobenzene 3-Hydroxynitrobenzene 3-Nitrophenol NSC 1551 Phenol, m-nitro- m-Hydroxynitrobenzene m-Nitrofenol m-Nitrophenol meta-Nitrophenol
Inchi:	InChI=1S/C6H5NO3/c8-6-3-1-2-5(4-6)7(9)10/h1-4,8H
InchiKey:	RTZZCYNQPHTPPL-UHFFFAOYSA-N
Formula:	C6H5NO3
SMILES:	O=[N+](O)c1cccc(O)c1
Mol. weight [g/mol]:	139.11
CAS:	554-84-7

Physical Properties

Property code	Value	Unit	Source
chs	-2870.00 ± 1.50	kJ/mol	NIST Webbook
chs	-2880.00	kJ/mol	NIST Webbook
chs	-2875.10 ± 0.90	kJ/mol	NIST Webbook
gf	-7.02	kJ/mol	Joback Method
hf	-105.50 ± 1.80	kJ/mol	NIST Webbook
hf	-109.30 ± 1.10	kJ/mol	NIST Webbook
hfs	-225.00	kJ/mol	NIST Webbook
hfs	-205.70 ± 1.70	kJ/mol	NIST Webbook
hfs	-200.50 ± 1.00	kJ/mol	NIST Webbook
hfus	22.48	kJ/mol	Joback Method
hsub	100.20 ± 0.60	kJ/mol	NIST Webbook
hsub	100.20 ± 0.60	kJ/mol	NIST Webbook
hsub	91.20 ± 0.50	kJ/mol	NIST Webbook
hsub	91.23 ± 0.49	kJ/mol	NIST Webbook
hvap	85.90	kJ/mol	NIST Webbook
ie	9.00	eV	NIST Webbook
ie	9.33	eV	NIST Webbook
log10ws	-1.01		Aqueous Solubility Prediction Method

log10ws	-1.01		Estimated Solubility Method
logp	1.300		Crippen Method
mcvol	94.930	ml/mol	McGowan Method
pc	5899.00	kPa	Joback Method
rinpol	1514.00		NIST Webbook
rinpol	1484.60		NIST Webbook
rinpol	1530.00		NIST Webbook
rinpol	1514.00		NIST Webbook
rinpol	1484.60		NIST Webbook
tb	595.82	K	Joback Method
tc	861.12	K	Joback Method
tf	370.10	K	Aqueous Solubility Prediction Method
vc	0.311	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	255.77	J/mol×K	816.90	Joback Method
cpg	261.56	J/mol×K	861.12	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
hfust	19.20	kJ/mol	370.00	NIST Webbook
hfust	21.30	kJ/mol	369.95	NIST Webbook
hfust	19.20	kJ/mol	370.00	NIST Webbook
hfust	18.06	kJ/mol	369.00	NIST Webbook
hfust	19.19	kJ/mol	371.20	NIST Webbook
hfust	19.19	kJ/mol	371.20	NIST Webbook
hsubt	91.60 ± 1.70	kJ/mol	330.50	NIST Webbook
hsubt	92.00 ± 2.00	kJ/mol	328.00	NIST Webbook
hsubt	98.50 ± 0.60	kJ/mol	321.00	NIST Webbook
hsubt	76.20	kJ/mol	319.50	NIST Webbook
sfust	57.60	J/mol×K	369.95	NIST Webbook
sfust	51.88	J/mol×K	370.00	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	467.20	K	9.30	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	9.89249e+00
Coeff. B	-2.32617e+03
Coeff. C	-7.71340e+01
Temperature range (K), min.	319.32
Temperature range (K), max.	584.92

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
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=C554847&Units=SI
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
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mccvol:	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
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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