Phenol, 4-methyl-2-nitro-

Other names:	2-Nitro-4-cresol
	2-Nitro-4-methylphenol
	2-Nitro-p-cresol
	4-Hydroxy-3-nitrotoluene
	4-Methyl-2-nitrophenol
	o-Nitro-p-cresol
	p-Cresol, 2-nitro-
Inchi:	InChI=1S/C7H7NO3/c1-5-2-3-7(9)6(4-5)8(10)11/h2-4,9H,1H3
InchiKey:	SYDNSSSQVSOXTN-UHFFFAOYSA-N
Formula:	C7H7NO3
SMILES:	Cc1ccc(O)c([N+](=O)[O-])c1
Mol. weight [g/mol]:	153.14
CAS:	119-33-5

Physical Properties

Property code	Value	Unit	Source
gf	-8.23	kJ/mol	Joback Method
hf	-150.82	kJ/mol	Joback Method
hfus	24.68	kJ/mol	Joback Method
hvap	63.72	kJ/mol	Joback Method
log10ws	-2.15		Crippen Method
logp	1.609		Crippen Method
mcvol	109.020	ml/mol	McGowan Method
pc	5008.59	kPa	Joback Method
rinpol	1250.00		NIST Webbook
rinpol	1260.00		NIST Webbook
rinpol	1236.40		NIST Webbook
rinpol	1236.40		NIST Webbook
rinpol	1249.80		NIST Webbook
rinpol	1249.80		NIST Webbook
rinpol	1241.30		NIST Webbook
ripol	1919.00		NIST Webbook
ripol	1914.00		NIST Webbook
ripol	1914.00		NIST Webbook
ripol	1922.00		NIST Webbook
ripol	1919.00		NIST Webbook
tb	623.68	K	Joback Method

tc	883.67	K	Joback Method
tf	462.92	K	Joback Method
vc	0.367	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	262.28	J/mol×K	623.68	Joback Method
cpg	271.81	J/mol×K	667.01	Joback Method
cpg	280.56	J/mol×K	710.34	Joback Method
cpg	288.66	J/mol×K	753.67	Joback Method
cpg	296.21	J/mol×K	797.01	Joback Method
cpg	303.32	J/mol×K	840.34	Joback Method
cpg	310.10	J/mol×K	883.67	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	398.20	K	2.90	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.01729e+01
Coeff. B	-2.52676e+03
Coeff. C	-8.42820e+01
Temperature range (K), min.	339.89
Temperature range (K), max.	604.05

Sources

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=C119335&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
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
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
pvap:	Vapor pressure
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume