Benzenamine, N-methyl-2-nitro-

Other names:	2-Nitro-N-methylaniline
	Aniline, N-methyl-o-nitro-
	N-Methyl-2-nitroaniline
	N-Methyl-o-nitroaniline
	o-(Methylamino)nitrobenzene
	o-Nitro-N-methyl aniline
Inchi:	InChI=1S/C7H8N2O2/c1-8-6-4-2-3-5-7(6)9(10)11/h2-5,8H,1H3
InchiKey:	KFBOUJZFFJDYTA-UHFFFAOYSA-N
Formula:	C7H8N2O2
SMILES:	CNc1ccccc1[N+](=O)[O-]
Mol. weight [g/mol]:	152.15
CAS:	612-28-2

Physical Properties

Property code	Value	Unit	Source
gf	235.78	kJ/mol	Joback Method
hf	79.96	kJ/mol	Joback Method
hfus	24.00	kJ/mol	Joback Method
hvap	57.14	kJ/mol	Joback Method
ie	8.02	eV	NIST Webbook
log10ws	-2.13		Crippen Method
logp	1.636		Crippen Method
mcvol	113.130	ml/mol	McGowan Method
pc	4167.71	kPa	Joback Method
tb	593.23	K	Joback Method
tc	841.00	K	Joback Method
tf	403.86	K	Joback Method
vc	0.436	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	263.79	J/mol×K	593.23	Joback Method
cpg	275.04	J/mol×K	634.53	Joback Method

cpg	285.42	J/mol×K	675.82	Joback Method
cpg	294.99	J/mol×K	717.12	Joback Method
cpg	303.78	J/mol×K	758.41	Joback Method
cpg	311.84	J/mol×K	799.71	Joback Method
cpg	319.22	J/mol×K	841.00	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.25107e+01
Coeff. B	-3.79209e+03
Coeff. C	-8.72810e+01
Temperature range (K), min.	397.52
Temperature range (K), max.	614.02

Sources

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C612282&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

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

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

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