Benzene, 1,2-dimethyl-4-nitro-

Other names:	1,2-Dimethyl-4-nitrobenzene
	3,4-Dimethyl-1-nitrobenzene
	3,4-Dimethylnitrobenzene
	4-Nitro-1,2-dimethylbenzene
	4-Nitro-o-xylene
	o-Xylene, 4-nitro-
	p-Nitro-o-xylene
	para-Nitro-ortho-xylene
Inchi:	InChI=1S/C8H9NO2/c1-6-3-4-8(9(10)11)5-7(6)2/h3-5H,1-2H3
InchiKey:	HFZKOYWDLDYELC-UHFFFAOYSA-N
Formula:	C8H9NO2
SMILES:	Cc1ccc([N+](=O)[O-])cc1C
Mol. weight [g/mol]:	151.16
CAS:	99-51-4

Physical Properties

Property code	Value	Unit	Source
ea	0.92 ± 0.05	eV	NIST Webbook
gf	145.18	kJ/mol	Joback Method
hf	-5.62	kJ/mol	Joback Method
hfus	21.10	kJ/mol	Joback Method
hvap	53.59	kJ/mol	Joback Method
log10ws	-3.07		Crippen Method
logp	2.212		Crippen Method
mcvol	117.240	ml/mol	McGowan Method
pc	3572.80	kPa	Joback Method
tb	570.92	K	Joback Method
tc	816.66	K	Joback Method
tf	301.70 ± 1.00	K	NIST Webbook
vc	0.458	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source

cpg	264.31	J/mol×K	570.92	Joback Method
cpg	276.23	J/mol×K	611.88	Joback Method
cpg	287.35	J/mol×K	652.83	Joback Method
cpg	297.69	J/mol×K	693.79	Joback Method
cpg	307.28	J/mol×K	734.75	Joback Method
cpg	316.17	J/mol×K	775.71	Joback Method
cpg	324.37	J/mol×K	816.66	Joback Method
hvapt	63.60	kJ/mol	467.50	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	416.20	K	2.70	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.56588e+01
Coeff. B	-4.74134e+03
Coeff. C	-8.68640e+01
Temperature range (K), min.	395.32
Temperature range (K), max.	545.08

Sources

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

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C99514&Units=SI

Legend

cpg:	Ideal gas heat capacity
ea:	Electron affinity
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
hvapt:	Enthalpy of vaporization at a given temperature
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
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume