Benzene, 1,2-dimethyl-3-nitro-

Other names:	1,2-Dimethyl-3-nitrobenzene
	2,3-Dimethylnitrobenzene
	3-Nitro-o-xylene
	o-Xylene, 3-nitro-
Inchi:	InChI=1S/C8H9NO2/c1-6-4-3-5-8(7(6)2)9(10)11/h3-5H,1-2H3
InchiKey:	FVHAWXWFPBPFOS-UHFFFAOYSA-N
Formula:	C8H9NO2
SMILES:	Cc1cccc([N+](=O)[O-])c1C
Mol. weight [g/mol]:	151.16
CAS:	83-41-0

Physical Properties

Property code	Value	Unit	Source
ea	0.92 ± 0.05	eV	NIST Webbook
ea	0.85 ± 0.10	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	518.20	K	NIST Webbook
tc	816.66	K	Joback Method
tf	287.40 ± 1.00	K	NIST Webbook
vc	0.458	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	316.17	J/mol×K	775.71	Joback Method
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	324.37	J/mol×K	816.66	Joback Method
hvapt	59.40	kJ/mol	450.50	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.45741e+01
Coeff. B	-4.32473e+03
Coeff. C	-8.38060e+01
Temperature range (K), min.	386.52
Temperature range (K), max.	550.71

Sources

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=C83410&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

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