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

Other names:	1,3-Dimethyl-2-nitrobenzene
	2,6-Dimethylnitrobenzene
	2-Nitro-1,3-dimethylbenzene
	2-Nitro-m-xylene
	m-Xylene, 2-nitro-
Inchi:	InChI=1S/C8H9NO2/c1-6-4-3-5-7(2)8(6)9(10)11/h3-5H,1-2H3
InchiKey:	HDFQKJQEWGVKCQ-UHFFFAOYSA-N
Formula:	C8H9NO2
SMILES:	Cc1cccc(C)c1[N+](=O)[O-]
Mol. weight [g/mol]:	151.16
CAS:	81-20-9

Physical Properties

Property code	Value	Unit	Source
chl	-4383.50 ± 0.70	kJ/mol	NIST Webbook
ea	2.61 ± 0.05	eV	NIST Webbook
ea	0.74 ± 0.09	eV	NIST Webbook
ea	0.81 ± 0.05	eV	NIST Webbook
gf	145.18	kJ/mol	Joback Method
hf	8.60 ± 1.60	kJ/mol	NIST Webbook
hfl	-50.80 ± 1.30	kJ/mol	NIST Webbook
hfus	21.10	kJ/mol	Joback Method
hvap	59.40 ± 0.90	kJ/mol	NIST Webbook
hvap	57.50 ± 0.80	kJ/mol	NIST Webbook
ie	9.17 ± 0.01	eV	NIST Webbook
ie	9.17	eV	NIST Webbook
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	288.00 ± 0.40	K	NIST Webbook
tf	288.55 ± 0.30	K	NIST Webbook
vc	0.458	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	307.28	J/mol×K	734.75	Joback Method
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	324.37	J/mol×K	816.66	Joback Method
hvapt	57.20 ± 0.80	kJ/mol	303.50	NIST Webbook
hvapt	49.70	kJ/mol	435.50	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	498.20	K	99.20	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.50126e+01
Coeff. B	-4.34986e+03
Coeff. C	-7.99140e+01
Temperature range (K), min.	375.32
Temperature range (K), max.	528.30

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C81209&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

chl:	Standard liquid enthalpy of combustion
cpg:	Ideal gas heat capacity
ea:	Electron affinity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfl:	Liquid phase 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
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
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume