Benzenamine, N,N-dimethyl-3-nitro-

Other names:	1-(Dimethylamino)-3-nitrobenzene
	3-Nitro-N,N-dimethylaniline
	Aniline, N,N-dimethyl-m-nitro-
	Benzene, 1-(dimethylamino)-3-nitro-
	N,N-Dimethyl-3-nitroaniline
	N,N-Dimethyl-m-nitroaniline
	NSC 9814
	m-Nitro-N,N-dimethylaniline
Inchi:	InChI=1S/C8H10N2O2/c1-9(2)7-4-3-5-8(6-7)10(11)12/h3-6H,1-2H3
InchiKey:	CJDICMLSLYHRPT-UHFFFAOYSA-N
Formula:	C8H10N2O2
SMILES:	CN(C)c1cccc([N+](=O)[O-])c1
Mol. weight [g/mol]:	166.18
CAS:	619-31-8

Physical Properties

Property code	Value	Unit	Source
affp	894.10	kJ/mol	NIST Webbook
basg	867.60	kJ/mol	NIST Webbook
chs	-4557.20 ± 1.50	kJ/mol	NIST Webbook
ea	0.98 ± 0.05	eV	NIST Webbook
gf	265.59	kJ/mol	Joback Method
hf	72.60 ± 1.80	kJ/mol	NIST Webbook
hfs	-20.10 ± 1.80	kJ/mol	NIST Webbook
hfus	24.51	kJ/mol	Joback Method
hsub	92.72 ± 0.27	kJ/mol	NIST Webbook
hsub	92.70 ± 0.30	kJ/mol	NIST Webbook
hvap	54.97	kJ/mol	Joback Method
log10ws	-2.03		Crippen Method
logp	1.661		Crippen Method
mcvol	127.220	ml/mol	McGowan Method
pc	3628.97	kPa	Joback Method
tb	555.70	K	NIST Webbook
tc	818.79	K	Joback Method
tf	333.65 ± 1.50	K	NIST Webbook
vc	0.475	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	299.59	J/mol×K	578.38	Joback Method
cpg	312.53	J/mol×K	618.45	Joback Method
cpg	324.50	J/mol×K	658.52	Joback Method
cpg	335.55	J/mol×K	698.59	Joback Method
cpg	345.73	J/mol×K	738.65	Joback Method
cpg	355.11	J/mol×K	778.72	Joback Method
cpg	363.72	J/mol×K	818.79	Joback Method
hvapt	52.30	kJ/mol	492.50	NIST Webbook
hvapt	48.20	kJ/mol	424.50	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.51369e+01
Coeff. B	-4.83938e+03
Coeff. C	-9.56210e+01
Temperature range (K), min.	421.52
Temperature range (K), max.	588.16

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=C619318&Units=SI

Legend

affp:	Proton affinity
basg:	Gas basicity
chs:	Standard solid 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
hfs:	Solid phase enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hsub:	Enthalpy of sublimation 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