Benzenamine, N,N-dimethyl-4-nitro-

Other names:	1-(Dimethylamino)-4-nitrobenzene
	4-(Dimethylamino)nitrobenzene
	4-Nitro-N,N-dimethylaniline
	4-Nitrodimethylaniline
	Aniline, N,N-dimethyl-p-nitro-
	N,N-Dimethyl-4-nitroaniline
	N,N-Dimethyl-4-nitrobenzenamine
	N,N-Dimethyl-p-nitroaniline
	NSC 9815
	p-(Dimethylamino)nitrobenzene
	p-Nitro-N,N-dimethylaniline
	p-Nitrodimethylaniline
Inchi:	InChI=1S/C8H10N2O2/c1-9(2)7-3-5-8(6-4-7)10(11)12/h3-6H,1-2H3
InchiKey:	QJAIOCKFIORVFU-UHFFFAOYSA-N
Formula:	C8H10N2O2
SMILES:	CN(C)c1ccc([N+](=O)[O-])cc1
Mol. weight [g/mol]:	166.18
CAS:	100-23-2

Physical Properties

Property code	Value	Unit	Source
affp	896.70	kJ/mol	NIST Webbook
basg	870.20	kJ/mol	NIST Webbook
chs	-4541.87 ± 0.94	kJ/mol	NIST Webbook
chs	-4538.70 ± 1.20	kJ/mol	NIST Webbook
gf	265.59	kJ/mol	Joback Method
hf	62.80 ± 2.60	kJ/mol	NIST Webbook
hf	67.30 ± 1.70	kJ/mol	NIST Webbook
hfs	-38.50 ± 1.60	kJ/mol	NIST Webbook
hfs	-35.40 ± 1.40	kJ/mol	NIST Webbook
hfus	24.51	kJ/mol	Joback Method
hsub	101.30 ± 2.00	kJ/mol	NIST Webbook
hsub	101.30 ± 2.00	kJ/mol	NIST Webbook
hsub	102.70 ± 1.00	kJ/mol	NIST Webbook
hsub	102.70 ± 1.10	kJ/mol	NIST Webbook
hvap	54.97	kJ/mol	Joback Method
ie	8.00	eV	NIST Webbook

ie	7.60 ± 0.10	eV	NIST Webbook
log10ws	-2.03		Crippen Method
logp	1.661		Crippen Method
mcvol	127.220	ml/mol	McGowan Method
pc	3628.97	kPa	Joback Method
tb	578.38	K	Joback Method
tc	818.79	K	Joback Method
tf	436.90 ± 1.00	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
hsubt	98.70 ± 1.70	kJ/mol	355.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.07012e+01
Coeff. B	-3.04507e+03
Coeff. C	-8.69330e+01
Temperature range (K), min.	379.35
Temperature range (K), max.	651.91

Sources

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=C100232&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

Legend

affp:	Proton affinity
basg:	Gas basicity
chs:	Standard solid enthalpy of combustion
cpg:	Ideal gas heat capacity
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
hsubt:	Enthalpy of sublimation at a given temperature
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