

Benzenamine, N,N-dimethyl-4-nitroso-

Other names:	Aniline, N,N-dimethyl-p-nitroso- p-(Dimethylamino)nitrosobenzene p-(N,N-Dimethylamino)nitrosobenzene p-Nitroso-N,N-dimethylaniline Accelerine Dimethyl(p-nitrosophenyl)amine N,N-Dimethyl-p-nitrosoaniline N,N-Dimethyl-4-nitrosoaniline NDMA Ultra Brilliant Blue P 4-(Dimethylamino)nitrosobenzene 4-Nitroso-N,N-dimethylaniline 4-Nitrosodimethylaniline p-Nitroso dimethylaniline p-Nitrosodimethylanilide NCI-C01821 Dimethyl-p-nitrosoaniline Paranitrosodimethylanilide UN 1369 Vulcaniline N,N-Dimethyl-4-nitrosobenzenamine NSC 2775
Inchi:	InChI=1S/C8H10N2O/c1-10(2)8-5-3-7(9-11)4-6-8/h3-6H,1-2H3
InchiKey:	CMEWLCATCRTSGF-UHFFFAOYSA-N
Formula:	C8H10N2O
SMILES:	CN(C)c1ccc(N=O)cc1
Mol. weight [g/mol]:	150.18
CAS:	138-89-6

Physical Properties

Property code	Value	Unit	Source
chs	-4680.20 ± 1.20	kJ/mol	NIST Webbook
chs	-4703.20	kJ/mol	NIST Webbook
hf	185.00 ± 2.30	kJ/mol	NIST Webbook
hfs	103.00 ± 1.60	kJ/mol	NIST Webbook
hsub	82.00 ± 1.70	kJ/mol	NIST Webbook

hsub	82.00 ± 1.70	kJ/mol	NIST Webbook
hvap	47.48	kJ/mol	Joback Method
ie	7.20	eV	NIST Webbook
ie	7.80 ± 0.10	eV	NIST Webbook
log10ws	-2.14		Crippen Method
logp	2.151		Crippen Method
mcvol	121.350	ml/mol	McGowan Method
pc	3501.28	kPa	Joback Method
tb	489.94	K	Joback Method
tc	696.16	K	Joback Method
tf	358.90 ± 0.70	K	NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cps	206.70	J/mol×K	293.00	NIST Webbook

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=C138896&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

chs:	Standard solid enthalpy of combustion
cps:	Solid phase heat capacity
hf:	Enthalpy of formation at standard conditions
hfs:	Solid phase enthalpy of formation at standard conditions
hsub:	Enthalpy of sublimation at standard conditions
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point

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