4'-DIMETHYLAMINO-3-NITROAZOBENZENE

Other names: Aniline, N,N-dimethyl-p-((m-nitrophenyl)azo)-
Benzenamine, N,N-dimethyl-4-((3-nitrophenyl)azo)-
N,N-Dimethyl-p-((m-nitrophenyl)azo)aniline
N,N-Dimethyl-4-((3-nitrophenyl)azo)aniline
3'-Nitro-4-dimethylaminoazobenzol (3'NO2-DAB)
3'-Nitro-4-((dimethylamino)azo)benzene
4-Dimethylamino-3' nitroazobenzene
Azobenzene, 4-dimethylamino-3'-nitro-
3-Nitro-4'-(N,N-dimethylamino)-azobenzene
3-Nitro-4'-dimethylaminoazobenzene
NSC 204512

Inchi: InChI=1S/C14H14N4O2/c1-17(2)13-8-6-11(7-9-13)15-16-12-4-3-5-14(10-12)18(19)20/h3

InchiKey: BISWHFCOHYEFQW-UHFFFAOYSA-N

Formula: C14H14N4O2

SMILES: CN(C)c1ccc(N=Nc2cccc([N+](=O)[O-])c2)cc1

Mol. weight [g/mol]: 270.29

Physical Properties

Property code	Value	Unit	Source
hf	349.71	kJ/mol	Cheméo Relay (1.0)
hvap	100.92	kJ/mol	Cheméo Relay (1.0)
ie	7.52	eV	Cheméo Relay (1.0)
log10ws	-4.87		Cheméo Relay (1.0)
logp	4.076		Crippen Method
mcvol	203.660	ml/mol	McGowan Method
tb	649.40	K	Cheméo Relay (1.0)
tf	422.76	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hsubt	133.90 ± 3.80	kJ/mol	400.00	NIST Webbook
hsubt	133.10 ± 3.80	kJ/mol	401.00	NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C3837556&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

hf:	Enthalpy of formation 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
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point