N,N'-Diethyl-m-nitroaniline

Other names: N,N-Diethyl-m-nitroaniline
Benzenamine, N,N-diethyl-3-nitro-
Inchi: InChI=1S/C10H14N2O2/c1-3-11(4-2)9-6-5-7-10(8-9)12(13)14/h5-8H,3-4H2,1-2H3
InchiKey: QSNHMSRICSDACJ-UHFFFAOYSA-N
Formula: C10H14N2O2
SMILES: CCN(CC)c1cccc([N+](=O)[O-])c1
Mol. weight [g/mol]: 194.23

Physical Properties

Property code	Value	Unit	Source
hf	-5.85	kJ/mol	Cheméo Relay (1.0)
hfus	29.69	kJ/mol	Joback Method
hvap	76.18	kJ/mol	Cheméo Relay (1.0)
ie	7.81	eV	Cheméo Relay (1.0)
log10ws	-3.51		Cheméo Relay (1.0)
logp	2.441		Crippen Method
mcvol	155.400	ml/mol	McGowan Method
tb	562.20	K	NIST Webbook
tf	327.25	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	394.46	J/mol×K	624.14	Joback Method
cpg	408.90	J/mol×K	662.60	Joback Method
cpg	422.31	J/mol×K	701.06	Joback Method
cpg	434.76	J/mol×K	739.52	Joback Method
cpg	446.29	J/mol×K	777.98	Joback Method
cpg	456.97	J/mol×K	816.44	Joback Method
cpg	466.85	J/mol×K	854.90	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	448.00 ± 1.00	K	2.40	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=C2216162&Units=SI

Joback Method: https://en.wikipedia.org/wiki/Joback_method

Legend

cpg: Ideal gas heat capacity

hf: Enthalpy of formation at standard conditions

hfus: Enthalpy of fusion 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

tb: Normal Boiling Point Temperature

tbrp: Boiling point at reduced pressure

tf: Normal melting (fusion) point