1,4-Benzenediamine, N,N-diethyl-

Other names:
p-Phenylenediamine, N,N-diethyl-
p-(Diethylamino)aniline
p-Amino-N,N-diethylaniline
p-Aminodiethylaniline
N,N-Diethyl-p-phenylenediamine
N,N-Diethyl-4-aminoaniline
4-(Diethylamino)aniline
4-Amino-N,N-diethylaniline
N,N-Diethyl-1,4-phenylenediamine
N,N-diethyl-p-phenylendiamine
Diethyl-p-phenylenediamine
Diethyl-para-phenylenediamine
DPD
1,4-Benzenediamine, N1,N1-diethyl-
N,N-Diethyl-1,4-benzenediamine
NSC 147488

Inchi: InChI=1S/C10H16N2/c1-3-12(4-2)10-7-5-9(11)6-8-10/h5-8H,3-4,11H2,1-2H3
InchiKey: QNGVNLMMEQUVQK-UHFFFAOYSA-N
Formula: C10H16N2
SMILES: CCN(CC)c1ccc(N)cc1
Mol. weight [g/mol]: 164.25
CAS: 93-05-0

Physical Properties

Property code	Value	Unit	Source
gf	313.33	kJ/mol	Joback Method
hf	76.65	kJ/mol	Joback Method
hfus	23.53	kJ/mol	Joback Method
hvap	53.48	kJ/mol	Joback Method
log10ws	-1.85		Crippen Method
logp	2.115		Crippen Method
mcvol	147.960	ml/mol	McGowan Method
pc	3062.55	kPa	Joback Method
rinpol	1429.60		NIST Webbook
rinpol	1429.60		NIST Webbook
tb	534.20	K	NIST Webbook
tc	758.53	K	Joback Method

tf	357.13	K	Joback Method
vc	0.534	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	350.77	J/mol×K	544.83	Joback Method
cpg	366.07	J/mol×K	580.45	Joback Method
cpg	380.44	J/mol×K	616.06	Joback Method
cpg	393.92	J/mol×K	651.68	Joback Method
cpg	406.56	J/mol×K	687.30	Joback Method
cpg	418.39	J/mol×K	722.91	Joback Method
cpg	429.45	J/mol×K	758.53	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	388.70	K	0.70	NIST Webbook

Sources

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=C93050&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions

hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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