1,2-Benzenediamine, N-phenyl-

Other names:	o-Phenylenediamine, N-phenyl-
	o-Aminodiphenylamine
	o-Semidine
	C.I. 50005
	N-Phenyl-o-Phenylenediamine
	2-Aminodiphenylamine
	N-Phenyl-1,2-phenylenediamine
Inchi:	InChI=1S/C12H12N2/c13-11-8-4-5-9-12(11)14-10-6-2-1-3-7-10/h1-9,14H,13H2
InchiKey:	NFCPRRWCTNLGSN-UHFFFAOYSA-N
Formula:	C12H12N2
SMILES:	Nc1ccccc1Nc1ccccc1
Mol. weight [g/mol]:	184.24
CAS:	534-85-0

Physical Properties

Property code	Value	Unit	Source
gf	421.19	kJ/mol	Joback Method
hf	257.84	kJ/mol	Joback Method
hfus	24.82	kJ/mol	Joback Method
hvap	64.60	kJ/mol	Joback Method
log10ws	-2.91		Crippen Method
logp	3.012		Crippen Method
mcvol	152.380	ml/mol	McGowan Method
pc	3659.77	kPa	Joback Method
tb	655.00	K	Joback Method
tc	910.40	K	Joback Method
tf	426.28	K	Joback Method
vc	0.555	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	384.08	J/mol×K	655.00	Joback Method
cpg	398.63	J/mol×K	697.57	Joback Method

cpg	411.93	J/mol×K	740.13	Joback Method
cpg	424.08	J/mol×K	782.70	Joback Method
cpg	435.16	J/mol×K	825.27	Joback Method
cpg	445.25	J/mol×K	867.84	Joback Method
cpg	454.44	J/mol×K	910.40	Joback Method

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=C534850&Units=SI

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
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume