Benzenamine, N-methyl-N-phenyl-

Other names:	Diphenylamine, N-methyl- Diphenylmethylamine Methyldiphenylamine N,N-Diphenylmethylamine N-METHYL DIPHENYLAMINE N-Methyl-N-phenylaniline N-Methyldiphenylamine NSC 3790
Inchi:	InChI=1S/C13H13N/c1-14(12-8-4-2-5-9-12)13-10-6-3-7-11-13/h2-11H,1H3
InchiKey:	DYFFAVRFJWYYQO-UHFFFAOYSA-N
Formula:	C13H13N
SMILES:	CN(c1ccccc1)c1ccccc1
Mol. weight [g/mol]:	183.25
CAS:	552-82-9

Physical Properties

Property code	Value	Unit	Source
chl	-7094.00 ± 7.10	kJ/mol	NIST Webbook
gf	394.18	kJ/mol	Joback Method
hf	228.94	kJ/mol	Joback Method
hfl	120.50 ± 7.10	kJ/mol	NIST Webbook
hfus	20.53	kJ/mol	Joback Method
hvap	51.13	kJ/mol	Joback Method
ie	6.94 ± 0.03	eV	NIST Webbook
ie	7.33	eV	NIST Webbook
log10ws	-3.18		Crippen Method
logp	3.455		Crippen Method
mcvol	156.490	ml/mol	McGowan Method
pc	3065.95	kPa	Joback Method
rinpol	1837.00		NIST Webbook
ripol	2450.00		NIST Webbook
ripol	2450.00		NIST Webbook
tb	566.55 ± 0.30	K	NIST Webbook
tb	569.15 ± 1.00	K	NIST Webbook
tc	803.09	K	Joback Method
tf	263.55 ± 0.20	K	NIST Webbook
vc	0.566	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	360.07	J/mol×K	562.64	Joback Method
cpg	377.74	J/mol×K	602.72	Joback Method
cpg	394.00	J/mol×K	642.79	Joback Method
cpg	408.93	J/mol×K	682.87	Joback Method
cpg	422.64	J/mol×K	722.94	Joback Method
cpg	435.20	J/mol×K	763.02	Joback Method
cpg	446.72	J/mol×K	803.09	Joback Method
cpl	301.20	J/mol×K	298.00	NIST Webbook
hvapt	65.20	kJ/mol	465.50	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.52885e+01
Coeff. B	-5.30882e+03
Coeff. C	-6.90130e+01
Temperature range (K), min.	422.91
Temperature range (K), max.	601.12

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	4.47419e+01
Coeff. B	-9.14336e+03
Coeff. C	-3.81908e+00
Coeff. D	1.55742e-06
Temperature range (K), min.	376.15
Temperature range (K), max.	555.15

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
KDB:	https://www.cheric.org/files/research/kdb/mol/mol1315.mol
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C552829&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
KDB Vapor Pressure Data:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1315
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

chl:	Standard liquid enthalpy of combustion
cpg:	Ideal gas heat capacity
cpl:	Liquid phase heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfl:	Liquid phase enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
hvapt:	Enthalpy of vaporization at a given temperature
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
pvap:	Vapor pressure
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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