N,N,N',N'-tetramethyl-p-phenylenediamine

Other names: 1,4-Benzenediamine, N,N,N',N'-tetramethyl-
Inchi: InChI=1S/C10H16N2/c1-11(2)9-5-7-10(8-6-9)12(3)4/h5-8H,1-4H3
InchiKey: CJAOGUFAAWZWNI-UHFFFAOYSA-N
Formula: C10H16N2
SMILES: CN(C)c1ccc(N(C)C)cc1
Mol. weight [g/mol]: 164.25
CAS: 100-22-1

Physical Properties

Property code	Value	Unit	Source
chs	-6261.30 ± 3.80	kJ/mol	NIST Webbook
gf	357.66	kJ/mol	Joback Method
hf	110.39	kJ/mol	Joback Method
hfs	39.60 ± 3.90	kJ/mol	NIST Webbook
hfus	21.35	kJ/mol	Joback Method
hvap	44.88	kJ/mol	Joback Method
ie	6.20 ± 0.02	eV	NIST Webbook
ie	6.70	eV	NIST Webbook
ie	6.75	eV	NIST Webbook
ie	6.20 ± 0.05	eV	NIST Webbook
ie	6.10 ± 0.10	eV	NIST Webbook
log10ws	-1.29		Crippen Method
logp	1.819		Crippen Method
mcvol	147.960	ml/mol	McGowan Method
pc	2871.95	kPa	Joback Method
tb	533.20	K	NIST Webbook
tc	685.33	K	Joback Method
tf	306.34	K	Joback Method
vc	0.523	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	322.36	J/mol×K	484.74	Joback Method

cpg	338.74	J/mol×K	518.17	Joback Method
cpg	354.17	J/mol×K	551.60	Joback Method
cpg	368.69	J/mol×K	585.03	Joback Method
cpg	382.34	J/mol×K	618.47	Joback Method
cpg	395.17	J/mol×K	651.90	Joback Method
cpg	407.21	J/mol×K	685.33	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C100221&Units=SI
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

Legend

chs:	Standard solid enthalpy of combustion
cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfs:	Solid phase 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
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume