

1,4-Benzenediamine, N,N,N',N'-tetramethyl-

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

Physical Properties

Property code	Value	Unit	Source
af	0.5322		Cheméo Relay (1.0)
chs	-6261.30 ± 3.80	kJ/mol	NIST Webbook
gf	357.66	kJ/mol	Joback Method
hf	82.97	kJ/mol	Cheméo Relay (1.0)
hfs	39.60 ± 3.90	kJ/mol	NIST Webbook
hfus	21.35	kJ/mol	Joback Method
hvap	68.82	kJ/mol	Cheméo Relay (1.0)
ie	6.10 ± 0.10	eV	NIST Webbook
ie	6.75	eV	NIST Webbook
ie	6.70	eV	NIST Webbook
ie	6.20 ± 0.02	eV	NIST Webbook
ie	6.20 ± 0.05	eV	NIST Webbook
log10ws	-2.96		Cheméo Relay (1.0)
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	736.70	K	Cheméo Relay (1.0)
tf	367.85	K	Cheméo Relay (1.0)

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

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=C100221&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

af:	Acentric Factor
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

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