

2,3,5,6-Tetramethyl-para-phenylenediamine

Other names:	2,3,5,6-Tetramethyl-p-phenylenediamine 1,4-Benzenediamine, 2,3,5,6-tetramethyl-
Inchi:	InChI=1S/C10H16N2/c1-5-6(2)10(12)8(4)7(3)9(5)11/h11-12H2,1-4H3
InchiKey:	WCZNKVPCIFMXEQ-UHFFFAOYSA-N
Formula:	C10H16N2
SMILES:	Cc1c(C)c(N)c(C)c(C)c1N
Mol. weight [g/mol]:	164.25
CAS:	3102-87-2

Physical Properties

Property code	Value	Unit	Source
gf	230.48	kJ/mol	Joback Method
hf	-2.97	kJ/mol	Joback Method
hfus	24.15	kJ/mol	Joback Method
hvap	64.72	kJ/mol	Joback Method
ie	8.63 ± 0.03	eV	NIST Webbook
ie	6.43	eV	NIST Webbook
log10ws	-2.64		Crippen Method
logp	2.085		Crippen Method
mcvol	147.960	ml/mol	McGowan Method
pc	3059.17	kPa	Joback Method
tb	624.84	K	Joback Method
tc	853.94	K	Joback Method
tf	422.15 ± 2.00	K	NIST Webbook
vc	0.545	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	371.77	J/molxK	624.84	Joback Method
cpg	385.11	J/molxK	663.02	Joback Method
cpg	397.75	J/molxK	701.21	Joback Method
cpg	409.69	J/molxK	739.39	Joback Method
cpg	420.95	J/molxK	777.57	Joback Method

cpg	431.53	J/mol×K	815.75	Joback Method
cpg	441.45	J/mol×K	853.94	Joback Method

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=C3102872&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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
hvac:	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

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