

1,3-BENZENEDIAMINE, N,N,N',N'-TETRAMETHYL-

Other names:	1,3-Phenylenediamine, N,N,N'-tetramethyl-N,N,N',N'-tetramethylbenzene-1,3-diamine
Inchi:	InChI=1S/C10H16N2/c1-11(2)9-6-5-7-10(8-9)12(3)4/h5-8H,1-4H3
InchiKey:	LFZLVJBOEONQHV-UHFFFAOYSA-N
Formula:	C10H16N2
SMILES:	CN(C)c1cccc(N(C)C)c1
Mol. weight [g/mol]:	164.25

Physical Properties

Property code	Value	Unit	Source
af	0.5230		Cheméo Relay (1.0)
gf	357.66	kJ/mol	Joback Method
hf	81.68	kJ/mol	Cheméo Relay (1.0)
hfus	21.35	kJ/mol	Joback Method
hvap	68.33	kJ/mol	Cheméo Relay (1.0)
ie	6.82	eV	Cheméo Relay (1.0)
log10ws	-2.84		Cheméo Relay (1.0)
logp	1.819		Crippen Method
mcvol	147.960	ml/mol	McGowan Method
pc	2871.95	kPa	Joback Method
rinpol	1504.00		NIST Webbook
tb	540.17	K	Cheméo Relay (1.0)
tc	733.62	K	Cheméo Relay (1.0)
tf	343.28	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

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
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=C22440933&Units=SI

Legend

af:	Acentric Factor
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
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point

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