2,4,6-Trimethyl-1,3-phenylenediamine

Other names:	2,4,6-Trimethyl-m-phenylenediamine 1,3-Benzenediamine, 2,4,6-trimethyl- m-Phenylenediamine,2,4,6-trimethyl- 2,4-Mesitylenediamine 2,4-Diamino-1,3,5-trimethylbenzene 1,3-Diamino-2,4,6-trimethylbenzene 2,4,6-Trimethyl-1,3-benzenediamine 2,4,6-trimethylbenzene-1,3-diamine
Inchi:	InChI=1S/C9H14N2/c1-5-4-6(2)9(11)7(3)8(5)10/h4H,10-11H2,1-3H3
InchiKey:	ZVDSMYGTJDFNHN-UHFFFAOYSA-N
Formula:	C9H14N2
SMILES:	Cc1cc(C)c(N)c(C)c1N
Mol. weight [g/mol]:	150.22
CAS:	3102-70-3

Physical Properties

Property code	Value	Unit	Source
gf	231.69	kJ/mol	Joback Method
hf	29.14	kJ/mol	Joback Method
hfus	21.95	kJ/mol	Joback Method
hvap	61.83	kJ/mol	Joback Method
log10ws	-2.17		Crippen Method
logp	1.776		Crippen Method
mcvol	133.870	ml/mol	McGowan Method
pc	3472.45	kPa	Joback Method
rinpol	1318.00		NIST Webbook
tb	596.98	K	Joback Method
tc	829.69	K	Joback Method
tf	434.21	K	Joback Method
vc	0.489	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source

cpg	325.25	J/mol×K	596.98	Joback Method
cpg	337.92	J/mol×K	635.76	Joback Method
cpg	349.89	J/mol×K	674.55	Joback Method
cpg	361.18	J/mol×K	713.33	Joback Method
cpg	371.79	J/mol×K	752.12	Joback Method
cpg	381.76	J/mol×K	790.90	Joback Method
cpg	391.09	J/mol×K	829.69	Joback Method

Sources

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=C3102703&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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
hvap:	Enthalpy of vaporization at standard conditions
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
vc:	Critical Volume