Benzenamine, 2,4,6-trimethyl-

Other names:	1-Amino-2,4,6-trimethylbenzene
	2,4,6-Trimethylaniline
	2,4,6-Trimethylbenzenamine
	2,4,6-Trimethylphenylamine
	2-Amino-1,3,5-trimethylbenzene
	2-Aminomesitylene
	Aminomesitylene
	Aniline, 2,4,6-trimethyl-
	Benzeneamine, 2,4,6-trimethyl-
	Mesidin
	Mesidine
	Mesitylamine
	Mesitylene, 2-amino-
Inchi:	InChI=1S/C9H13N/c1-6-4-7(2)9(10)8(3)5-6/h4-5H,10H2,1-3H3
InchiKey:	KWVPRPSXBZNOHS-UHFFFAOYSA-N
Formula:	C9H13N
SMILES:	Cc1cc(C)c(N)c(C)c1
Mol. weight [g/mol]:	135.21
CAS:	88-05-1

Physical Properties

Property code	Value	Unit	Source
gf	174.87	kJ/mol	Joback Method
hf	6.82	kJ/mol	Joback Method
hfus	17.14	kJ/mol	Joback Method
hvap	50.53	kJ/mol	Joback Method
ie	7.24	eV	NIST Webbook
ie	7.15	eV	NIST Webbook
log10ws	-2.53		Crippen Method
logp	2.194		Crippen Method
mcvol	123.890	ml/mol	McGowan Method
pc	3306.75	kPa	Joback Method
rinpol	1261.00		NIST Webbook
rinpol	214.41		NIST Webbook
rinpol	214.41		NIST Webbook
rinpol	1230.90		NIST Webbook
rinpol	1261.00		NIST Webbook

rinpol	1242.20		NIST Webbook
tb	505.70	K	NIST Webbook
tc	742.49	K	Joback Method
tf	268.25 ± 0.40	K	NIST Webbook
vc	0.461	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	271.32	J/mol×K	519.47	Joback Method
cpg	284.27	J/mol×K	556.64	Joback Method
cpg	296.55	J/mol×K	593.81	Joback Method
cpg	308.17	J/mol×K	630.98	Joback Method
cpg	319.16	J/mol×K	668.15	Joback Method
cpg	329.53	J/mol×K	705.32	Joback Method
cpg	339.30	J/mol×K	742.49	Joback Method
hvapt	64.10	kJ/mol	425.50	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.48394e+01
Coeff. B	-4.33350e+03
Coeff. C	-8.17210e+01
Temperature range (K), min.	379.52
Temperature range (K), max.	536.54

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C88051&Units=SI

The Yaws Handbook of Vapor Pressure: https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

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

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
hvapt:	Enthalpy of vaporization at a given temperature
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
pvap:	Vapor pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume