Benzenamine, 2,4,5-trimethyl-

Other names:	1,2,4-Trimethyl-5-aminobenzene
	1-Amino-2,4,5-trimethylbenzene
	2,4,5-Trimethylanilin
	2,4,5-Trimethylaniline
	2,4,5-Trimethylbenzenamine
	2,4,5-Trimethylphenylamine
	Aniline, 2,4,5-trimethyl-
	NCI-C02299
	NSC 37004
	Pseudocumidine
	Pseudokumidin
	psi-Cumidine
	«psi»-Cumidine
	Â«psiÂ»-Cumidine
Inchi:	InChI=1S/C9H13N/c1-6-4-8(3)9(10)5-7(6)2/h4-5H,10H2,1-3H3
InchiKey:	BMIPMKQAAJKBKP-UHFFFAOYSA-N
Formula:	C9H13N
SMILES:	Cc1cc(C)c(N)cc1C
Mol. weight [g/mol]:	135.21
CAS:	137-17-7

Physical Properties

Property code	Value	Unit	Source
chs	-5318.70	kJ/mol	NIST Webbook
gf	174.87	kJ/mol	Joback Method
hf	6.82	kJ/mol	Joback Method
hfs	-110.00	kJ/mol	NIST Webbook
hfus	17.14	kJ/mol	Joback Method
hvap	50.53	kJ/mol	Joback Method
log10ws	-2.53		Crippen Method
logp	2.194		Crippen Method
mcvol	123.890	ml/mol	McGowan Method
pc	3306.75	kPa	Joback Method
rinpol	220.25		NIST Webbook
tb	507.70	K	NIST Webbook
tc	742.49	K	Joback Method
tf	338.43	K	Joback Method

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

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.48428e+01
Coeff. B	-4.34972e+03
Coeff. C	-8.22770e+01
Temperature range (K), min.	341.15
Temperature range (K), max.	538.64

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=C137177&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

Legend

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
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