Benzenamine, N,N-diethyl-3-methyl-

Other names:	1-(Diethylamino)-3-methylbenzene
	3-(Diethylamino)-1-methylbenzene
	3-(Diethylamino)toluene
	3-(N,N-Diethylamino)toluene
	3-Methyl-N,N-diethylbenzenamine
	N,N-Diethyl-3-methylaniline
	N,N-Diethyl-m-toluidine
	NSC 96629
	m-Methyl(diethylamino)benzene
	m-Methyl-N,N-diethylaniline
	m-Toluidine, N,N-diethyl-
Inchi:	InChI=1S/C11H17N/c1-4-12(5-2)11-8-6-7-10(3)9-11/h6-9H,4-5H2,1-3H3
InchiKey:	CIPVVROJHKLHJI-UHFFFAOYSA-N
Formula:	C11H17N
SMILES:	CCN(CC)c1cccc(C)c1
Mol. weight [g/mol]:	163.26
CAS:	91-67-8

Physical Properties

Property code	Value	Unit	Source
affp	964.10	kJ/mol	NIST Webbook
basg	932.20	kJ/mol	NIST Webbook
gf	255.30	kJ/mol	Joback Method
hf	22.22	kJ/mol	Joback Method
hfus	20.92	kJ/mol	Joback Method
hvap	45.06	kJ/mol	Joback Method
ie	6.90	eV	NIST Webbook
log10ws	-2.69		Crippen Method
logp	2.841		Crippen Method
mcvol	152.070	ml/mol	McGowan Method
pc	2603.08	kPa	Joback Method
rinpol	1290.10		NIST Webbook
rinpol	1290.10		NIST Webbook
tb	495.18	K	Joback Method
tc	695.71	K	Joback Method
tf	285.14	K	Joback Method
vc	0.561	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	334.22	J/mol×K	495.18	Joback Method
cpg	350.65	J/mol×K	528.60	Joback Method
cpg	366.18	J/mol×K	562.02	Joback Method
cpg	380.85	J/mol×K	595.44	Joback Method
cpg	394.69	J/mol×K	628.86	Joback Method
cpg	407.74	J/mol×K	662.29	Joback Method
cpg	420.04	J/mol×K	695.71	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.47193e+01
Coeff. B	-4.29023e+03
Coeff. C	-8.14430e+01
Temperature range (K), min.	378.72
Temperature range (K), max.	537.47

Sources

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

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C91678&Units=SI

Legend

affp:	Proton affinity
basg:	Gas basicity
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
pvap:	Vapor pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume