Benzenamine, N,N-diethyl-4-methyl-

Other names:	4-(Diethylamino)toluene
	4-Methyl-N,N-diethylbenzenamine
	N,N-Diethyl-4-methylaniline
	N,N-Diethyl-4-toluidine
	N,N-Diethyl-p-toluidine
	p-Methyl-N,N-diethylaniline
	p-Toluidine, N,N-diethyl-
Inchi:	InChI=1S/C11H17N/c1-4-12(5-2)11-8-6-10(3)7-9-11/h6-9H,4-5H2,1-3H3
InchiKey:	HKJNHYJTVPWVGV-UHFFFAOYSA-N
Formula:	C11H17N
SMILES:	CCN(CC)c1ccc(C)cc1
Mol. weight [g/mol]:	163.26
CAS:	613-48-9

Physical Properties

Property code	Value	Unit	Source
affp	962.80	kJ/mol	NIST Webbook
basg	931.00	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	6.81 ± 0.05	eV	NIST Webbook
ie	6.84	eV	NIST Webbook
ie	6.93	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	1342.70		NIST Webbook
rinpol	1343.20		NIST Webbook
rinpol	1342.70		NIST Webbook
ripol	1708.70		NIST Webbook
ripol	1709.30		NIST Webbook
ripol	1708.70		NIST Webbook
ripol	1708.70		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

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	401.00 ± 2.00	K	2.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.45196e+01
Coeff. B	-4.21228e+03
Coeff. C	-8.07480e+01
Temperature range (K), min.	376.72
Temperature range (K), max.	538.20

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C613489&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

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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume