

Benzenamine, N-ethyl-2-methyl-

Other names:	1-(Ethylamino)-2-methylbenzene 2-(Ethylamino)toluene N-Ethyl-2-methylaniline N-Ethyl-2-methylbenzenamine N-Ethyl-2-toluidine N-Ethyl-N-(2-methylphenyl)amine N-Ethyl-o-toluidine NSC 8888 o-Methyl-N-ethylaniline o-Toluidine, N-ethyl-
Inchi:	InChI=1S/C9H13N/c1-3-10-9-7-5-4-6-8(9)2/h4-7,10H,3H2,1-2H3
InchiKey:	MWOUGPLLVEUMM-UHFFFAOYSA-N
Formula:	C9H13N
SMILES:	CCNc1ccccc1C
Mol. weight [g/mol]:	135.21
CAS:	94-68-8

Physical Properties

Property code	Value	Unit	Source
gf	217.07	kJ/mol	Joback Method
hf	49.44	kJ/mol	Joback Method
hfus	17.82	kJ/mol	Joback Method
hvap	45.00	kJ/mol	Joback Method
log10ws	-2.37		Crippen Method
logp	2.427		Crippen Method
mcvol	123.890	ml/mol	McGowan Method
pc	3254.14	kPa	Joback Method
tb	491.20	K	NIST Webbook
tc	697.80	K	Joback Method
tf	282.79	K	Joback Method
vc	0.467	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	260.77	J/mol×K	487.15	Joback Method
cpg	274.66	J/mol×K	522.26	Joback Method
cpg	287.77	J/mol×K	557.37	Joback Method
cpg	300.15	J/mol×K	592.47	Joback Method
cpg	311.81	J/mol×K	627.58	Joback Method
cpg	322.79	J/mol×K	662.69	Joback Method
cpg	333.12	J/mol×K	697.80	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	368.70	K	1.30	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.46471e+01
Coeff. B	-4.15256e+03
Coeff. C	-7.71340e+01
Temperature range (K), min.	366.32
Temperature range (K), max.	521.94

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=C94688&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/ci9903071
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
hvac:	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
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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