

Benzenamine, N-ethyl-3-methyl-

Other names:	N-Ethyl-3-methylaniline N-Ethyl-3-methylbenzenamine N-Ethyl-N-(3-methylphenyl)amine N-Ethyl-m-toluidine N-Ethyl-meta-toluidine NSC 8624 m-Methyl-N-ethylaniline m-Toluidine, N-ethyl-
Inchi:	InChI=1S/C9H13N/c1-3-10-9-6-4-5-8(2)7-9/h4-7,10H,3H2,1-2H3
InchiKey:	GUYMMHOQXYZMJQ-UHFFFAOYSA-N
Formula:	C9H13N
SMILES:	CCNc1cccc(C)c1
Mol. weight [g/mol]:	135.21
CAS:	102-27-2

Physical Properties

Property code	Value	Unit	Source
chl	-5370.00 ± 2.30	kJ/mol	NIST Webbook
gf	217.07	kJ/mol	Joback Method
hf	30.50 ± 3.80	kJ/mol	NIST Webbook
hfl	-29.50 ± 2.30	kJ/mol	NIST Webbook
hfus	17.82	kJ/mol	Joback Method
hvap	60.00 ± 3.00	kJ/mol	NIST Webbook
hvap	60.00	kJ/mol	NIST Webbook
hvap	60.00 ± 3.00	kJ/mol	NIST Webbook
log10ws	-2.37		Crippen Method
logp	2.427		Crippen Method
mcvol	123.890	ml/mol	McGowan Method
pc	3254.14	kPa	Joback Method
rinpol	1200.00		NIST Webbook
rinpol	1200.00		NIST Webbook
ripol	1802.00		NIST Webbook
ripol	1802.00		NIST Webbook
tb	494.20	K	NIST Webbook
tc	697.80	K	Joback Method
tf	282.79	K	Joback Method
vc	0.467	m ³ /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

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.48193e+01
Coeff. B	-4.24029e+03
Coeff. C	-7.85240e+01
Temperature range (K), min.	370.32
Temperature range (K), max.	524.50

Sources

McGowan Method:

<http://link.springer.com/article/10.1007/BF02311772>

NIST Webbook:

<http://webbook.nist.gov/cgi/cbook.cgi?ID=C102272&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

Joback Method:

https://en.wikipedia.org/wiki/Joback_method

Legend

chl:	Standard liquid enthalpy of combustion
cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfl:	Liquid 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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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