Aniline, 3-ethyl-

Other names:	3-C2H5C6H4NH2
	3-Ethylaniline
	Aniline, m-ethyl-
	Benzenamine, 3-ethyl-
	m-Ethylaniline
Inchi:	InChI=1S/C8H11N/c1-2-7-4-3-5-8(9)6-7/h3-6H,2,9H2,1H3
InchiKey:	AMKPQMFZCBTTAT-UHFFFAOYSA-N
Formula:	C8H11N
SMILES:	CCc1cccc(N)c1
Mol. weight [g/mol]:	121.18
CAS:	587-02-0

Physical Properties

Property code	Value	Unit	Source
affp	897.90	kJ/mol	NIST Webbook
basg	866.10	kJ/mol	NIST Webbook
gf	185.71	kJ/mol	Joback Method
hf	50.40	kJ/mol	Joback Method
hfus	15.32	kJ/mol	Joback Method
hvap	46.98	kJ/mol	Joback Method
log10ws	-1.91		Crippen Method
logp	1.831		Crippen Method
mcvol	109.800	ml/mol	McGowan Method
pc	3843.54	kPa	Joback Method
rinpol	1141.00		NIST Webbook
rinpol	1141.00		NIST Webbook
ripol	1924.30		NIST Webbook
ripol	1924.30		NIST Webbook
tb	485.20	K	NIST Webbook
tb	487.00 ± 1.00	K	NIST Webbook
tc	710.97	K	Joback Method
tf	302.12	K	Joback Method
vc	0.405	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	228.77	J/mol×K	486.63	Joback Method
cpg	241.38	J/mol×K	524.02	Joback Method
cpg	253.24	J/mol×K	561.41	Joback Method
cpg	264.37	J/mol×K	598.80	Joback Method
cpg	274.81	J/mol×K	636.19	Joback Method
cpg	284.60	J/mol×K	673.58	Joback Method
cpg	293.75	J/mol×K	710.97	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	367.20	K	0.80	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.49758e+01
Coeff. B	-4.23229e+03
Coeff. C	-7.65780e+01
Temperature range (K), min.	364.72
Temperature range (K), max.	514.51

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=C587020&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
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