Benzenamine, 4-ethyl-

Other names:	1-Amino-4-ethylbenzene
	4-Aminoethylbenzene
	4-ETHYLANILINE
	4-ETHYLBENZENAMIINE
	4-Ethylphenylamine
	Aniline, 4-ethyl-
	Aniline, p-ethyl-
	NSC 62015
	P-AMINOETHYLBENZENE
	p-Ethylaminobenzene
	p-Ethylaniline
	para-Ethylaniline
Inchi:	InChI=1S/C8H11N/c1-2-7-3-5-8(9)6-4-7/h3-6H,2,9H2,1H3
InchiKey:	HRXZRAXKKNUKRF-UHFFFAOYSA-N
Formula:	C8H11N
SMILES:	CCc1ccc(N)cc1
Mol. weight [g/mol]:	121.18
CAS:	589-16-2

Physical Properties

Property code	Value	Unit	Source
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
ie	7.60 ± 0.10	eV	NIST Webbook
log10ws	-1.91		Crippen Method
logp	1.831		Crippen Method
mcvol	109.800	ml/mol	McGowan Method
pc	3843.54	kPa	Joback Method
ripol	1947.00		NIST Webbook
ripol	1893.70		NIST Webbook
ripol	1919.90		NIST Webbook
ripol	1947.00		NIST Webbook
tb	490.70	K	NIST Webbook
tb	488.00 ± 4.00	K	NIST Webbook
tb	485.00 ± 6.00	K	NIST Webbook

tb	490.37 ± 0.07	K	NIST Webbook
tb	489.00 ± 3.00	K	NIST Webbook
tb	489.20	K	NIST Webbook
tc	710.97	K	Joback Method
tf	268.60 ± 2.00	K	NIST Webbook
tf	264.20 ± 5.00	K	NIST Webbook
tf	268.20 ± 4.00	K	NIST Webbook
tf	267.72 ± 0.05	K	NIST Webbook
tf	267.30 ± 2.00	K	NIST Webbook
tf	268.00 ± 0.02	K	NIST Webbook
vc	0.405	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	274.81	J/mol×K	636.19	Joback Method
cpg	284.60	J/mol×K	673.58	Joback Method
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	293.75	J/mol×K	710.97	Joback Method
hvapt	53.10	kJ/mol	442.00	NIST Webbook
hvapt	54.60	kJ/mol	407.50	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	364.50 ± 0.50	K	0.80	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)

Coeff. A	1.49557e+01
Coeff. B	-4.25329e+03
Coeff. C	-7.75510e+01
Temperature range (K), min.	367.52
Temperature range (K), max.	518.57

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	1.53556e+02
Coeff. B	-1.31932e+04
Coeff. C	-2.00942e+01
Coeff. D	1.01886e-05
Temperature range (K), min.	393.15
Temperature range (K), max.	491.15

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C589162&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
KDB Vapor Pressure Data:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1304
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
KDB:	https://www.cheric.org/files/research/kdb/mol/mol1304.mol
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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
hvap:	Enthalpy of vaporization at standard conditions
hvapt:	Enthalpy of vaporization at a given temperature
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
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