Benzenamine, 2-ethyl-

Other names:	2-ETHYLANILINE
	2-ETHYLBENZENAMINE
	2-Ethylbenzeneamine
	2-Ethylphenylamine
	Aniline, 2-ethyl-
	Aniline, o-ethyl-
	NSC 62014
	O-AMINOETHYLBENZENE
	O-ETHYLANILINE
	UN 2273
	ortho-Ethylaniline
Inchi:	InChI=1S/C8H11N/c1-2-7-5-3-4-6-8(7)9/h3-6H,2,9H2,1H3
InchiKey:	MLPVBIWIRCKMJV-UHFFFAOYSA-N
Formula:	C8H11N
SMILES:	CCc1ccccc1N
Mol. weight [g/mol]:	121.18
CAS:	578-54-1

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	60.60 ± 0.90	kJ/mol	NIST Webbook
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
rinpol	1119.00		NIST Webbook
rinpol	1124.10		NIST Webbook
ripol	1848.00		NIST Webbook
ripol	1902.00		NIST Webbook
ripol	1902.00		NIST Webbook
tb	487.00 ± 5.00	K	NIST Webbook
tb	482.70 ± 1.00	K	NIST Webbook
tb	482.70	K	NIST Webbook

tb	487.00 ± 4.00	K	NIST Webbook
tb	487.00 ± 4.00	K	NIST Webbook
tc	710.97	K	Joback Method
tf	263.20 ± 20.00	K	NIST Webbook
tf	226.60 ± 1.00	K	NIST Webbook
vc	0.405	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
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	274.81	J/mol×K	636.19	Joback Method
cpg	293.75	J/mol×K	710.97	Joback Method
hvapt	60.30 ± 0.90	kJ/mol	303.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.47984e+01
Coeff. B	-4.14709e+03
Coeff. C	-7.53270e+01
Temperature range (K), min.	361.12
Temperature range (K), max.	512.46

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	8.09753e+01
Coeff. B	-9.66120e+03
Coeff. C	-9.23402e+00
Coeff. D	3.02507e-06

Temperature range (K), min.	226.55
Temperature range (K), max.	704.00

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C578541&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=1302
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/mol1302.mol

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
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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