Benzenamine, 2-ethoxy-

Other names:	2-AMINOPHENETOLE
	2-ETHOXYBENZENAMINE
	2-Ethoxyaniline
	2-Phenetidine
	O-ETHOXYANILINE
	UN 2311
	o-Aminophenetole
	o-Phenetidine
Inchi:	InChI=1S/C8H11NO/c1-2-10-8-6-4-3-5-7(8)9/h3-6H,2,9H2,1H3
InchiKey:	ULHFFAFDSSHFDA-UHFFFAOYSA-N
Formula:	C8H11NO
SMILES:	CCOc1ccccc1N
Mol. weight [g/mol]:	137.18
CAS:	94-70-2

Physical Properties

Property code	Value	Unit	Source
gf	80.71	kJ/mol	Joback Method
hf	-81.82	kJ/mol	Joback Method
hfus	16.51	kJ/mol	Joback Method
hvap	49.39	kJ/mol	Joback Method
log10ws	-1.64		Crippen Method
logp	1.667		Crippen Method
mcvol	115.670	ml/mol	McGowan Method
pc	3763.78	kPa	Joback Method
rinpol	1206.80		NIST Webbook
tb	505.70	K	NIST Webbook
tb	505.65 ± 0.50	K	NIST Webbook
tc	730.98	K	Joback Method
tf	324.35	K	Joback Method
vc	0.422	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	251.29	J/mol×K	509.05	Joback Method
cpg	263.62	J/mol×K	546.04	Joback Method
cpg	275.28	J/mol×K	583.03	Joback Method
cpg	286.30	J/mol×K	620.01	Joback Method
cpg	296.69	J/mol×K	657.00	Joback Method
cpg	306.45	J/mol×K	693.99	Joback Method
cpg	315.60	J/mol×K	730.98	Joback Method
hvapt	57.30	kJ/mol	415.50	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	400.70	K	1.90	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.73221e+01
Coeff. B	-6.21092e+03
Coeff. C	-1.67940e+01
Temperature range (K), min.	381.40
Temperature range (K), max.	533.92

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	2.12495e+01
Coeff. B	-7.03241e+03
Coeff. C	-4.28858e-01
Coeff. D	2.09166e-07
Temperature range (K), min.	373.15
Temperature range (K), max.	458.15

Sources

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/mol1480.mol
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C94702&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=1480
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
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
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume