Ethanol, 2-[(phenylmethyl)amino]-

Other names:	(N-Benzylamino)ethanol
	2-(Benzylamino)ethanol
	2-benzylaminoethanol
	Benzylaminoethanol
	Benzylethanolamine
	Ethanol, 2-(benzylamino)-
	N-Benzyl-N-ethanolamine
	N-benzylethanolamine
	NSC 11271
Inchi:	InChI=1S/C9H13NO/c11-7-6-10-8-9-4-2-1-3-5-9/h1-5,10-11H,6-8H2
InchiKey:	XNIOWJUQPMKCIJ-UHFFFAOYSA-N
Formula:	C9H13NO
SMILES:	OCCNCc1ccccc1
Mol. weight [g/mol]:	151.21
CAS:	104-63-2

Physical Properties

Property code	Value	Unit	Source
gf	89.88	kJ/mol	Joback Method
hf	-91.32	kJ/mol	Joback Method
hfus	22.29	kJ/mol	Joback Method
hvap	74.50	kJ/mol	NIST Webbook
log10ws	-1.64		Crippen Method
logp	0.768		Crippen Method
mcvol	129.760	ml/mol	McGowan Method
pc	3690.97	kPa	Joback Method
rinpol	1349.00		NIST Webbook
rinpol	1349.00		NIST Webbook
tb	574.35	K	Joback Method
tc	770.35	K	Joback Method
tf	331.09	K	Joback Method
vc	0.485	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	373.53	J/mol×K	770.35	Joback Method
cpg	364.93	J/mol×K	737.68	Joback Method
cpg	355.77	J/mol×K	705.02	Joback Method
cpg	346.03	J/mol×K	672.35	Joback Method
cpg	335.66	J/mol×K	639.68	Joback Method
cpg	324.64	J/mol×K	607.02	Joback Method
cpg	312.95	J/mol×K	574.35	Joback Method
hvapt	71.70	kJ/mol	328.00	NIST Webbook
pvap	0.24	kPa	362.91	Experimental vapor pressures of 1,2-bis(dimethylamino)ethane, 1-methylmorpholine, 1,2-bis(2-aminoethoxy)ethane and N-benzylethanolamine between 273.18 and 364.97K
pvap	0.11	kPa	352.92	Experimental vapor pressures of 1,2-bis(dimethylamino)ethane, 1-methylmorpholine, 1,2-bis(2-aminoethoxy)ethane and N-benzylethanolamine between 273.18 and 364.97K
pvap	0.03	kPa	332.89	Experimental vapor pressures of 1,2-bis(dimethylamino)ethane, 1-methylmorpholine, 1,2-bis(2-aminoethoxy)ethane and N-benzylethanolamine between 273.18 and 364.97K
pvap	0.03	kPa	332.88	Experimental vapor pressures of 1,2-bis(dimethylamino)ethane, 1-methylmorpholine, 1,2-bis(2-aminoethoxy)ethane and N-benzylethanolamine between 273.18 and 364.97K

pvap	5.20e-03	kPa	312.85	Experimental vapor pressures of 1,2-bis(dimethylamino)ethane, 1-methylmorpholine, 1,2-bis(2-aminoethoxy)ethane and N-benzylethanolamine between 273.18 and 364.97K
pvap	7.82e-04	kPa	292.82	Experimental vapor pressures of 1,2-bis(dimethylamino)ethane, 1-methylmorpholine, 1,2-bis(2-aminoethoxy)ethane and N-benzylethanolamine between 273.18 and 364.97K
pvap	0.23	kPa	362.91	Experimental vapor pressures of 1,2-bis(dimethylamino)ethane, 1-methylmorpholine, 1,2-bis(2-aminoethoxy)ethane and N-benzylethanolamine between 273.18 and 364.97K

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	427.70	K	1.60	NIST Webbook

Sources

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=C104632&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Experimental vapor pressures of 1,2-bis(dimethylamino)ethane, 1-methylmorpholine, 1,2-bis(2-aminoethoxy)ethane and N-benzylethanolamine between 273.18 and 364.97K	https://www.doi.org/10.1016/j.fluid.2009.04.006
Investigation of the isothermal (vapour + liquid) equilibria of aqueous 2-amino-2-methyl-1-propanol (AMP), N-benzylethanolamine, or 3-dimethylamino-1-propanol solutions at several temperatures:	https://www.doi.org/10.1016/j.jct.2010.04.015

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