

Ethanol, 2-(phenylamino)-

Other names:	Ethanol, 2-anilino- «beta»-Anilinoethanol Benzenamine, N-(2-hydroxyethyl)- N-(«beta»-Hydroxyethyl)aniline N-(2-Hydroxyethyl)aniline N-(2-Hydroxyethyl)phenylamine N-Phenylethanolamine 2-(Phenylamino)ethanol 2-Anilinoethanol N-Hydroxyethylaniline («beta»-Hydroxyethyl)aniline Aniline, N-(«beta»-hydroxyethyl)- Aniline, N-(2-hydroxyethyl)- Emery 5700 NSC 8393
Inchi:	InChI=1S/C8H11NO/c10-7-6-9-8-4-2-1-3-5-8/h1-5,9-10H,6-7H2
InchiKey:	MWGATWIBSKHFMR-UHFFFAOYSA-N
Formula:	C8H11NO
SMILES:	OCCNc1ccccc1
Mol. weight [g/mol]:	137.18
CAS:	122-98-5

Physical Properties

Property code	Value	Unit	Source
gf	81.46	kJ/mol	Joback Method
hf	-70.68	kJ/mol	Joback Method
hfus	19.70	kJ/mol	Joback Method
hvap	58.79	kJ/mol	Joback Method
log10ws	-1.16		Crippen Method
logp	1.091		Crippen Method
mcvol	115.670	ml/mol	McGowan Method
pc	4162.33	kPa	Joback Method
rinpol	1347.00		NIST Webbook
tb	559.20	K	NIST Webbook
tc	750.17	K	Joback Method
tf	319.82	K	Joback Method
vc	0.429	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	315.59	J/mol×K	717.06	Joback Method
cpg	267.41	J/mol×K	551.47	Joback Method
cpg	278.28	J/mol×K	584.59	Joback Method
cpg	288.50	J/mol×K	617.70	Joback Method
cpg	298.11	J/mol×K	650.82	Joback Method
cpg	307.13	J/mol×K	683.94	Joback Method
cpg	323.52	J/mol×K	750.17	Joback Method
hvapt	69.90	kJ/mol	465.00	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	424.20	K	1.30	NIST Webbook
tbrp	440.20	K	2.30	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=C122985&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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
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

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