

Ethanol, 2,2'-(phenylimino)bis-

Other names:	2,2'-(Phenylamino)diethanol
	2,2'-(Phenylimino)diethanol
	Di(hydroxyethyl)aniline
	Diethanolaminobenzene
	Diethanolaniline
	Diethanolphenylamine
	Emery 5703
	Ethanol, 2,2'-(phenylimino)di-
	N,N-Bis(2-hydroxyethyl)aniline
	N,N-Bis(«beta»-hydroxyethyl)aniline
	N,N-Bis(Â«betaÂ»-hydroxyethyl)aniline
	N,N-Di(2-hydroxyethyl)aniline
	N,N-Di(«beta»-hydroxyethyl)aniline
	N,N-Di(Â«betaÂ»-hydroxyethyl)aniline
	N,N-Diethanolaniline
	N,N-Dihydroxyethylaniline
	N,N-Dioxyethylaniline
	N-Phenyl-2,2'-iminodiethanol
	N-Phenyl-N,N-diethanolamine
	N-Phenyldiethanolamine
	NSC 6327
	Phenylbis(2-hydroxyethyl)amine
	Phenyldiethanolamine
	[Bis(2-hydroxyethyl)amino]benzene
Inchi:	InChI=1S/C10H15NO2/c12-8-6-11(7-9-13)10-4-2-1-3-5-10/h1-5,12-13H,6-9H2
InchiKey:	OJPDDQSCZGTACX-UHFFFAOYSA-N
Formula:	C10H15NO2
SMILES:	OCCN(CCO)c1ccccc1
Mol. weight [g/mol]:	181.23
CAS:	120-07-0

Physical Properties

Property code	Value	Unit	Source
gf	-17.13	kJ/mol	Joback Method
hf	-250.13	kJ/mol	Joback Method
hfus	26.89	kJ/mol	Joback Method

hvap	75.53	kJ/mol	Joback Method
log10ws	-0.73		Aqueous Solubility Prediction Method
logp	0.478		Crippen Method
mcvol	149.720	ml/mol	McGowan Method
pc	3607.21	kPa	Joback Method
tb	651.68	K	Joback Method
tc	833.32	K	Joback Method
tf	382.99	K	Joback Method
vc	0.543	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	447.61	J/mol×K	803.05	Joback Method
cpg	399.85	J/mol×K	651.68	Joback Method
cpg	410.57	J/mol×K	681.95	Joback Method
cpg	420.67	J/mol×K	712.23	Joback Method
cpg	430.20	J/mol×K	742.50	Joback Method
cpg	439.16	J/mol×K	772.78	Joback Method
cpg	455.58	J/mol×K	833.32	Joback Method
hvapt	77.60	kJ/mol	514.50	NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C120070&Units=SI>

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>

Joback Method: https://en.wikipedia.org/wiki/Joback_method

Aqueous Solubility Prediction Method: <http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDataset002.xlsx>

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
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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