

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

Joback Method:

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

Aqueous Solubility Prediction Method:

<http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa>

McGowan Method:

<http://link.springer.com/article/10.1007/BF02311772>

NIST Webbook:

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

Crippen Method:

<http://pubs.acs.org/doi/abs/10.1021/ci9903071>

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
hvac:	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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