

Benzenamine, 4,4'-(1,2-ethanediyl)bis-

Other names:	«alpha», «alpha»'-Bi-p-toluidine Aniline, 4,4'-ethylenedi- 1,2-Bis(p-aminophenyl)ethane 1,2-Bis(4-aminophenyl)ethane 4,4'-Diaminobibenzyl 4,4'-Ethylenedianiline 4,4-Ethylenedianiline Aniline, p,p'-ethylenedi- 4,4'-Ethylenebis(aniline) 4,4'-Diaminodibenzyl NSC 44062 NSC 580 NSC 60033
Inchi:	InChI=1S/C14H16N2/c15-13-7-3-11(4-8-13)1-2-12-5-9-14(16)10-6-12/h3-10H,1-2,15-16H
InchiKey:	UHNUHZHQLCGZDA-UHFFFAOYSA-N
Formula:	C14H16N2
SMILES:	<chem>Nc1ccc(CCc2ccc(N)cc2)cc1</chem>
Mol. weight [g/mol]:	212.29
CAS:	621-95-4

Physical Properties

Property code	Value	Unit	Source
gf	405.46	kJ/mol	Joback Method
hf	185.41	kJ/mol	Joback Method
hfus	29.71	kJ/mol	Joback Method
hvap	73.92	kJ/mol	Joback Method
ie	7.45 ± 0.05	eV	NIST Webbook
ie	7.60 ± 0.10	eV	NIST Webbook
log10ws	-3.16		Crippen Method
logp	2.636		Crippen Method
mcvol	180.560	ml/mol	McGowan Method
pc	3032.27	kPa	Joback Method
tb	728.10	K	Joback Method
tc	981.12	K	Joback Method
tf	491.94	K	Joback Method
vc	0.661	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	493.46	J/mol×K	728.10	Joback Method
cpg	508.37	J/mol×K	770.27	Joback Method
cpg	522.07	J/mol×K	812.44	Joback Method
cpg	534.63	J/mol×K	854.61	Joback Method
cpg	546.15	J/mol×K	896.78	Joback Method
cpg	556.69	J/mol×K	938.95	Joback Method
cpg	566.35	J/mol×K	981.12	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C621954&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
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
ie:	Ionization energy
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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