Benzenamine, 4,4'-methylenebis-

Other names:

4,4'-Diaminodiphenylmethan
4,4'-Diaminodiphenylmethane
4,4'-Diphenylmethanediamine
4,4'-Methylenebis(benzeneamine)
4,4'-Methylenebis[aniline]
4,4'-Methylenedianiline
4,4'-Methylenedibenzenamine
4,4'-methylenebisbenzenamine
4,4'-methylenedianilin
4,4-Methylenedianiline
4-(4-Aminobenzyl)aniline
Ancamine TL
Aniline, 4,4'-methylenedi-
Araldite hardener 972
Bis(4-aminophenyl)methane
Bis(aminophenyl)methane
Bis(p-aminophenyl)methane
Bis-p-aminofenylmethan
Curithane
DADPM
DDM
Di(4-aminophenyl)methane
Diaminodiphenylmethane
Dianiline, 4,4'-methylene-
Dianilinemethane
Epicure DDM
Epikure DDM
HT 972
Jeffamine AP-20
MDA
Methylenebis[aniline]
Methylenedianiline
NCI-C54604
NSC 4709
Sumicure M
Tonox
UN 2651
di-(p-aminophenyl)methane
p,p'-Diaminodifenylmethan
p,p'-Diaminodiphenylmethane

p,p'-Methylenedianiline
p-Toluidine, «alpha»-(p-aminophenyl)-
p-Toluidine, Â«alphaÂ»-(p-aminophenyl)-

Inchi: InChI=1S/C13H14N2/c14-12-5-1-10(2-6-12)9-11-3-7-13(15)8-4-11/h1-8H,9,14-15H2
InchiKey: YBRVSVVVWCFQMG-UHFFFAOYSA-N
Formula: C13H14N2
SMILES: Nc1ccc(Cc2ccc(N)cc2)cc1
Mol. weight [g/mol]: 198.26
CAS: 101-77-9

Physical Properties

Property code	Value	Unit	Source
gf	397.04	kJ/mol	Joback Method
hf	206.05	kJ/mol	Joback Method
hfus	27.12	kJ/mol	Joback Method
hvap	71.69	kJ/mol	Joback Method
ie	7.20	eV	NIST Webbook
ie	7.75 ± 0.05	eV	NIST Webbook
log10ws	-2.30		Aqueous Solubility Prediction Method
logp	2.442		Crippen Method
mcvol	166.470	ml/mol	McGowan Method
pc	3380.21	kPa	Joback Method
tb	705.22	K	Joback Method
tc	964.17	K	Joback Method
tf	363.70 ± 0.50	K	NIST Webbook
tf	366.00	K	NIST Webbook
tf	363.80 ± 0.50	K	NIST Webbook
tf	364.40	K	Aqueous Solubility Prediction Method
tf	366.00	K	NIST Webbook
vc	0.606	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	502.58	J/mol×K	921.01	Joback Method

cpg	469.32	J/mol×K	791.54	Joback Method
cpg	481.43	J/mol×K	834.70	Joback Method
cpg	492.49	J/mol×K	877.85	Joback Method
cpg	511.79	J/mol×K	964.17	Joback Method
cpg	441.64	J/mol×K	705.22	Joback Method
cpg	456.08	J/mol×K	748.38	Joback Method
hfust	9.23	kJ/mol	363.70	NIST Webbook
hfust	9.23	kJ/mol	363.70	NIST Webbook
hfust	19.69	kJ/mol	362.70	NIST Webbook
hfust	9.22	kJ/mol	363.70	NIST Webbook
hvapt	100.60	kJ/mol	508.00	NIST Webbook
hvapt	89.00 ± 2.00	kJ/mol	471.00	NIST Webbook
hvapt	98.00	kJ/mol	515.50	NIST Webbook
hvapt	109.30	kJ/mol	368.00	NIST Webbook
sfust	25.40	J/mol×K	363.70	NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C101779&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Measurement and Correlation of the Solubility for 4,4'-Diaminodiphenylmethane in Different Solvents:	https://www.doi.org/10.1021/je501111d
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

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
hfust:	Enthalpy of fusion at a given temperature
hvap:	Enthalpy of vaporization at standard conditions
hvapt:	Enthalpy of vaporization at a given temperature
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume

pc:	Critical Pressure
sfust:	Entropy of fusion at a given temperature
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume