

2-(4-Aminophenyl)ethylamine

Other names:	4-Amino-«beta»-phenylethylamine Benzeneethanamine, 4-amino- «beta»-[4-Aminophenyl]ethylamine 4-(2-aminoethyl)aniline
Inchi:	InChI=1S/C8H12N2/c9-6-5-7-1-3-8(10)4-2-7/h1-4H,5-6,9-10H2
InchiKey:	LNPMZQXEPNWCMG-UHFFFAOYSA-N
Formula:	C8H12N2
SMILES:	NCCc1ccc(N)cc1
Mol. weight [g/mol]:	136.19
CAS:	13472-00-9

Physical Properties

Property code	Value	Unit	Source
gf	252.16	kJ/mol	Joback Method
hf	84.19	kJ/mol	Joback Method
hfus	20.52	kJ/mol	Joback Method
hvap	57.62	kJ/mol	Joback Method
log10ws	-1.34		Crippen Method
logp	0.770		Crippen Method
mcvol	119.780	ml/mol	McGowan Method
pc	4130.29	kPa	Joback Method
tb	559.16	K	Joback Method
tc	793.38	K	Joback Method
tf	385.38	K	Joback Method
vc	0.433	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	281.99	J/molxK	559.16	Joback Method
cpg	294.53	J/molxK	598.20	Joback Method
cpg	306.24	J/molxK	637.23	Joback Method
cpg	317.17	J/molxK	676.27	Joback Method
cpg	327.34	J/molxK	715.31	Joback Method

cpg	336.81	J/mol×K	754.34	Joback Method
cpg	345.59	J/mol×K	793.38	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	376.20	K	0.04	NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C13472009&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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
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
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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