Benzenepropanamine, «alpha»-methyl-

Other names:	3-Amino-1-phenylbutane
	«alpha»-Methylbenzenepropanamine
	1-Methyl-3-phenylpropylamine
	1-Phenyl-3-aminobutane
	4-Phenyl-2-aminobutane
	Propylamine, 1-methyl-3-phenyl-
	3-Phenyl-1-methylpropylamine
	Propylamine, «alpha»-methyl-«gamma»-phenyl-
	1-Phenyl-3-amino-butan
	«alpha»-Methyl-«gamma»-phenyl-N-propylamine
	2-Amino-4-phenylbutane
	NSC 115524
Inchi:	InChI=1S/C10H15N/c1-9(11)7-8-10-5-3-2-4-6-10/h2-6,9H,7-8,11H2,1H3
InchiKey:	WECUIGDEWBNQJJ-UHFFFAOYSA-N
Formula:	C10H15N
SMILES:	CC(N)CCc1ccccc1
Mol. weight [g/mol]:	149.23
CAS:	22374-89-6

Physical Properties

Property code	Value	Unit	Source
gf	209.74	kJ/mol	Joback Method
hf	15.31	kJ/mol	Joback Method
hfus	17.37	kJ/mol	Joback Method
hvap	50.38	kJ/mol	Joback Method
log10ws	-2.66		Crippen Method
logp	1.966		Crippen Method
mcvol	137.980	ml/mol	McGowan Method
pc	3149.09	kPa	Joback Method
rinpol	1221.70		NIST Webbook
rinpol	1257.00		NIST Webbook
rinpol	1221.70		NIST Webbook
rinpol	1257.00		NIST Webbook
ripol	1724.00		NIST Webbook
ripol	1724.00		NIST Webbook
tb	494.70	K	NIST Webbook
tc	747.64	K	Joback Method

tf	297.14	K	Joback Method
vc	0.510	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	316.47	J/mol×K	526.97	Joback Method
cpg	331.87	J/mol×K	563.75	Joback Method
cpg	346.31	J/mol×K	600.53	Joback Method
cpg	359.84	J/mol×K	637.30	Joback Method
cpg	372.49	J/mol×K	674.08	Joback Method
cpg	384.32	J/mol×K	710.86	Joback Method
cpg	395.35	J/mol×K	747.64	Joback Method

Sources

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
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C22374896&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
rinpol: Non-polar retention indices
ripol: Polar retention indices

tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume