alpha.-Methylbenzylamine

Other names:	Benzenemethanamine, «alpha»-methyl-, (.+/-.)- Benzylamine, «alpha»-methyl-, (.+/-.)- (.+/-.)-«alpha»-Methylbenzylamine (.+/-.)-«alpha»-Phenylethylamine (.+/-.)-1-Phenethylamine (.+/-.)-1-Phenylethylamine DL-«alpha»-Phenylethylamine DL-1-Phenylethylamine Benzenemethanamine, «alpha»-methyl-, (±)- Benzylamine, «alpha»-methyl-, (±)- 1-Amino-1-phenylethane 1-Phenylethylamine Benzenemethanamine, «alpha»-methyl- DL-«alpha»-Methylbenzylamine Ethanamine, 1-phenyl- NSC 8391
Inchi:	InChI=1S/C8H11N/c1-7(9)8-5-3-2-4-6-8/h2-7H,9H2,1H3
InchiKey:	RQEUFEKYXDPUSK-UHFFFAOYSA-N
Formula:	C8H11N
SMILES:	CC(N)c1ccccc1
Mol. weight [g/mol]:	121.18
CAS:	618-36-0

Physical Properties

Property code	Value	Unit	Source
gf	192.90	kJ/mol	Joback Method
hf	56.59	kJ/mol	Joback Method
hfus	12.19	kJ/mol	Joback Method
hvap	54.50 ± 0.10	kJ/mol	NIST Webbook
log10ws	-2.17		Crippen Method
logp	1.706		Crippen Method
mcvol	109.800	ml/mol	McGowan Method
pc	3955.54	kPa	Joback Method
tb	481.21	K	Joback Method
tc	709.62	K	Joback Method
tf	274.60	K	Joback Method
vc	0.399	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	228.83	J/mol×K	481.21	Joback Method
cpg	242.28	J/mol×K	519.28	Joback Method
cpg	254.86	J/mol×K	557.35	Joback Method
cpg	266.60	J/mol×K	595.41	Joback Method
cpg	277.54	J/mol×K	633.48	Joback Method
cpg	287.73	J/mol×K	671.55	Joback Method
cpg	297.20	J/mol×K	709.62	Joback Method
hvapt	36.70	kJ/mol	305.00	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	458.20	K	101.00	NIST Webbook

Sources

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=C618360&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

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