Benzeneethanamine, 4-methoxy-

Other names:	Phenethylamine, p-methoxy-
	p-Methoxyphenethylamine
	p-Methoxyphenylethylamine
	Homoanisylamine
	Tyramine, O-methyl-
	2-(p-Methoxyphenyl)ethylamine
	2-(4-Methoxyphenyl)ethylamine
	4-Methoxy-«beta»-phenylethylamine
	4-Methoxy-2-phenethylamine
	4-Methoxybenzeneethanamine
	4-Methoxyphenethylamine
	4-Methoxyphenylethylamine
	USAF EL-52
	NSC 43687
Inchi:	InChI=1S/C9H13NO/c1-11-9-4-2-8(3-5-9)6-7-10/h2-5H,6-7,10H2,1H3
InchiKey:	LTPVSOCPYWDIFU-UHFFFAOYSA-N
Formula:	C9H13NO
SMILES:	COc1ccc(CCN)cc1
Mol. weight [g/mol]:	151.21
CAS:	55-81-2

Physical Properties

Property code	Value	Unit	Source
gf	89.13	kJ/mol	Joback Method
hf	-102.46	kJ/mol	Joback Method
hfus	19.10	kJ/mol	Joback Method
hvap	51.62	kJ/mol	Joback Method
ie	8.16 ± 0.08	eV	NIST Webbook
log10ws	-1.83		Crippen Method
logp	1.196		Crippen Method
mcvol	129.760	ml/mol	McGowan Method
pc	3356.75	kPa	Joback Method
rinpol	1318.80		NIST Webbook
tb	531.93	K	Joback Method
tc	750.09	K	Joback Method
tf	335.62	K	Joback Method
vc	0.478	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	295.02	J/mol×K	531.93	Joback Method
cpg	308.41	J/mol×K	568.29	Joback Method
cpg	321.08	J/mol×K	604.65	Joback Method
cpg	333.04	J/mol×K	641.01	Joback Method
cpg	344.32	J/mol×K	677.37	Joback Method
cpg	354.92	J/mol×K	713.73	Joback Method
cpg	364.86	J/mol×K	750.09	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	412.20	K	2.70	NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C55812&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
rinpol:	Non-polar retention indices
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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