Benzeneethanamine, 4-methoxy-«alpha»-methyl-

Other names: «alpha»-Methyl-«beta»-(p-methoxyphenyl)ethylamine
Phenethylamine, p-methoxy-«alpha»-methyl-
1-p-Methoxyphenyl-2-aminopropane
1-p-Methoxyphenyl-2-propylamine
Benzenethanamine,4-methoxy-«alpha»-methyl-(.+/-.)-
Phenethylamine, p-methoxy-«alpha»-methyl-, (.+/-.)-
Benzeneethanamine, 4-methoxy-«alpha»-methyl-, (.+/-.)-
(.+/-.)-p-Methoxyamphetamine
p-Methoxyamphetamine
4-Methoxyamphetamine
(.+/-.)-p-Methoxy-«alpha»-methylphenethylamine
PMA
1-(4-Methoxyphenyl)-2-propanamine
Paramethoxyamphetamine
(.+/-.)-1-(p-Methoxyphenyl)-2-aminopropane
(.+/-.)-4-Methoxyamphetamine
2-Amino-1-(4'-methoxyphenyl)propane
DL-p-Methoxy-«alpha»-methylphenethylamine
NSC 32757
p-Methoxy-«alpha»-methylphenethylamine
1-(4-methoxybenzyl)ethylamine

Inchi: InChI=1S/C10H15NO/c1-8(11)7-9-3-5-10(12-2)6-4-9/h3-6,8H,7,11H2,1-2H3

InchiKey: NEGYEDYHPHMHGK-UHFFFAOYSA-N

Formula: C10H15NO

SMILES: COc1ccc(CC(C)N)cc1

Mol. weight [g/mol]: 165.23

CAS: 23239-32-9

Physical Properties

Property code	Value	Unit	Source
gf	95.11	kJ/mol	Joback Method
hf	-128.38	kJ/mol	Joback Method
hfus	18.17	kJ/mol	Joback Method
hvap	53.46	kJ/mol	Joback Method
ie	8.16 ± 0.06	eV	NIST Webbook
log10ws	-2.36		Crippen Method

logp	1.585		Crippen Method
mcvol	143.850	ml/mol	McGowan Method
pc	3038.96	kPa	Joback Method
rinpol	1385.00		NIST Webbook
rinpol	1403.40		NIST Webbook
rinpol	1385.00		NIST Webbook
rinpol	1385.00		NIST Webbook
rinpol	1385.00		NIST Webbook
tb	554.37	K	Joback Method
tc	773.57	K	Joback Method
tf	331.89	K	Joback Method
vc	0.528	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	340.96	J/mol×K	554.37	Joback Method
cpg	355.65	J/mol×K	590.90	Joback Method
cpg	369.53	J/mol×K	627.44	Joback Method
cpg	382.60	J/mol×K	663.97	Joback Method
cpg	394.90	J/mol×K	700.51	Joback Method
cpg	406.43	J/mol×K	737.04	Joback Method
cpg	417.22	J/mol×K	773.57	Joback Method

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=C23239329&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
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
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume