

Phenethylamine, p-methoxy-«alpha»-methyl-, hydrochloride

Other names:	p-Methoxy-«alpha»-methylphenethylamine hydrochloride «beta»-p-Methoxyphenylisopropylaminhydrochlorid Phenethylamine, 4-methoxy-alpha-methyl-, hydrochloride 2-Propanamine, 1-(4-methoxyphenyl)-, hydrochloride
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.ClH
SMILES:	COc1ccc(CC(C)N)cc1
Mol. weight [g/mol]:	201.69
CAS:	3706-26-1

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
log10ws	-2.36		Crippen Method
logp	1.585		Crippen Method
mcvol	143.850	ml/mol	McGowan Method
pc	3038.96	kPa	Joback Method
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/molxK	554.37	Joback Method
cpg	355.65	J/molxK	590.90	Joback Method
cpg	369.53	J/molxK	627.44	Joback Method
cpg	382.60	J/molxK	663.97	Joback Method
cpg	394.90	J/molxK	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

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C3706261&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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
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
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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