Benzeneethanamine, 4-methoxy-N,«alpha»-dimethyl-

Other names: Phenethylamine, N,«alpha»-dimethyl-4-methoxy-
«alpha»-(4-Methoxyphenyl)-«beta»-methylaminopropane
1-(p-Methoxyphenyl)-2-methylaminopropane
Phenethylamine, p-methoxy-N,«alpha»-dimethyl-
1-(4-Methoxyphenyl)-2-methylamino-propan
1-(4-Methoxyphenyl)-N-methyl-2-propanamine
1-(4-Methoxyphenyl)-2-methylamino-propane
Methamphetamine, 4-methoxy
p-Methoxymethamphetamine
p-methoxy-N,«alpha»-dimethylphenethylamine

Inchi: InChI=1S/C11H17NO/c1-9(12-2)8-10-4-6-11(13-3)7-5-10/h4-7,9,12H,8H2,1-3H3

InchiKey: UGFMBZYKVQSQFX-UHFFFAOYSA-N

Formula: C11H17NO

SMILES: CNC(C)Cc1ccc(OC)cc1

Mol. weight [g/mol]: 179.26

CAS: 22331-70-0

Physical Properties

Property code	Value	Unit	Source
gf	126.47	kJ/mol	Joback Method
hf	-129.34	kJ/mol	Joback Method
hfus	20.66	kJ/mol	Joback Method
hvap	51.48	kJ/mol	Joback Method
log10ws	-2.53		Crippen Method
logp	1.846		Crippen Method
mcvol	157.940	ml/mol	McGowan Method
pc	2619.09	kPa	Joback Method
rinpol	1482.70		NIST Webbook
rinpol	1482.70		NIST Webbook
rinpol	1445.00		NIST Webbook
rinpol	1445.00		NIST Webbook
tb	554.89	K	Joback Method
tc	761.71	K	Joback Method
tf	312.56	K	Joback Method
vc	0.591	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	376.82	J/mol×K	554.89	Joback Method
cpg	392.50	J/mol×K	589.36	Joback Method
cpg	407.36	J/mol×K	623.83	Joback Method
cpg	421.41	J/mol×K	658.30	Joback Method
cpg	434.67	J/mol×K	692.77	Joback Method
cpg	447.17	J/mol×K	727.24	Joback Method
cpg	458.92	J/mol×K	761.71	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=C22331700&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
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume