Benzeneethanamine, 3,4-dimethoxy-

Other names:	Phenethylamine, 3,4-dimethoxy- «beta»-(3,4-Dimethoxyphenyl)ethylamine DIMPEA DMPE DMPEA Homoveratrylamine 2-(3,4-Dimethoxyphenyl)ethylamine 3,4-Dimethoxybenzeneethanamine 3,4-Dimethoxyphenethylamine Benzenethanamine, 3,4-dimethoxy- 3,4-Dimethoxyphenylethylamine Dimethoxydopamine Dimethoxyphenylethylamine Dopamine dimethyl ether 3,4-Dimethoxy-«beta»-phenethylamine 3,4-Dimethoxy-«beta»-phenylethylamine 3,4-Dimethoxyphenylethylamine(base) 3,4-Di-O-methyldopamine O,O-Dimethyldopamine 3,4-Dimethoxypheneethylamine Dimethylmescaline NSC 16948
Inchi:	InChI=1S/C10H15NO2/c1-12-9-4-3-8(5-6-11)7-10(9)13-2/h3-4,7H,5-6,11H2,1-2H3
InchiKey:	ANOUKFYBOAKOIR-UHFFFAOYSA-N
Formula:	C10H15NO2
SMILES:	COc1ccc(CCN)cc1OC
Mol. weight [g/mol]:	181.23
CAS:	120-20-7

Physical Properties

Property code	Value	Unit	Source
gf	-17.08	kJ/mol	Joback Method
hf	-266.79	kJ/mol	Joback Method
hfus	22.49	kJ/mol	Joback Method
hvap	56.92	kJ/mol	Joback Method
ie	8.03 ± 0.16	eV	NIST Webbook

ie	7.40	eV	NIST Webbook
ie	8.03	eV	NIST Webbook
log10ws	-1.95		Crippen Method
logp	1.205		Crippen Method
mcvol	149.720	ml/mol	McGowan Method
pc	2909.25	kPa	Joback Method
rinpol	1551.00		NIST Webbook
tb	582.21	K	Joback Method
tc	795.30	K	Joback Method
tf	381.64	K	Joback Method
vc	0.552	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	364.65	J/mol×K	582.21	Joback Method
cpg	378.45	J/mol×K	617.72	Joback Method
cpg	391.58	J/mol×K	653.24	Joback Method
cpg	404.04	J/mol×K	688.75	Joback Method
cpg	415.81	J/mol×K	724.27	Joback Method
cpg	426.90	J/mol×K	759.78	Joback Method
cpg	437.30	J/mol×K	795.30	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	461.20	K	2.00	NIST Webbook
tbrp	460.50 ± 0.50	K	2.00	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=C120207&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
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