Benzenethanamine, 3,4-dimethoxy-«alpha»-methyl-

Other names: Benzeneethanamine, 3,4-dimethoxy-«alpha»-methyl-
Phenethylamine, 3,4-dimethoxy-«alpha»-methyl-
3,4-Dimethoxyamphetamine
3,4-Dimethoxy-«alpha»-methylphenethylamine
3,4-Dimethoxyphenylisopropylamine
«alpha»-Methylhomoveratrylamine
DMA (3-4)

Inchi: InChI=1S/C11H17NO2/c1-8(12)6-9-4-5-10(13-2)11(7-9)14-3/h4-5,7-8H,6,12H2,1-3H3

InchiKey: KAZPHAGSWZTKDW-UHFFFAOYSA-N

Formula: C11H17NO2

SMILES: COc1ccc(CC(C)N)cc1OC

Mol. weight [g/mol]: 195.26

CAS: 120-26-3

Physical Properties

Property code	Value	Unit	Source
gf	-11.10	kJ/mol	Joback Method
hf	-292.71	kJ/mol	Joback Method
hfus	21.56	kJ/mol	Joback Method
hvap	58.75	kJ/mol	Joback Method
ie	8.03 ± 0.06	eV	NIST Webbook
log10ws	-2.48		Crippen Method
logp	1.593		Crippen Method
mcvol	163.810	ml/mol	McGowan Method
pc	2651.56	kPa	Joback Method
rinpol	1537.00		NIST Webbook
rinpol	1537.00		NIST Webbook
rinpol	1580.00		NIST Webbook
rinpol	1537.00		NIST Webbook
tb	604.65	K	Joback Method
tc	818.55	K	Joback Method
tf	377.91	K	Joback Method
vc	0.603	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	413.34	J/mol×K	604.65	Joback Method
cpg	428.28	J/mol×K	640.30	Joback Method
cpg	442.45	J/mol×K	675.95	Joback Method
cpg	455.85	J/mol×K	711.60	Joback Method
cpg	468.48	J/mol×K	747.25	Joback Method
cpg	480.33	J/mol×K	782.90	Joback Method
cpg	491.41	J/mol×K	818.55	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C120263&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
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume