4-ethyl-2,5-dimethoxy-«beta»-phenethylamine-M, (-COOH N-acetyl), methyl

Inchi: InChI=1S/C14H19NO5/c1-9(16)15-6-5-10-7-13(19-3)11(14(17)20-4)8-12(10)18-2/h7-8H,
InchiKey: ZQINOUKYNVCRBR-UHFFFAOYSA-N
Formula: C14H19NO5
SMILES: COC(=O)c1cc(OC)c(CCNC(C)=O)cc1OC
Mol. weight [g/mol]: 281.30

Physical Properties

Property code	Value	Unit	Source
gf	-332.93	kJ/mol	Joback Method
hf	-698.52	kJ/mol	Joback Method
hfus	36.75	kJ/mol	Joback Method
hvap	78.18	kJ/mol	Joback Method
log10ws	-2.56		Crippen Method
logp	1.169		Crippen Method
mcvol	215.090	ml/mol	McGowan Method
pc	2088.84	kPa	Joback Method
rinpol	2600.00		NIST Webbook
tb	786.51	K	Joback Method
tc	993.58	K	Joback Method
tf	530.73	K	Joback Method
vc	0.812	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	618.36	J/mol×K	786.51	Joback Method
cpg	631.61	J/mol×K	821.02	Joback Method
cpg	643.89	J/mol×K	855.53	Joback Method
cpg	655.19	J/mol×K	890.05	Joback Method
cpg	665.47	J/mol×K	924.56	Joback Method
cpg	674.74	J/mol×K	959.07	Joback Method
cpg	682.97	J/mol×K	993.58	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R514184&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

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