4-ethyl-2,5-dimethoxy-«beta»-phenethylamine-M, (OH-N-acetyl-), isomer 2, propionylated

Inchi: InChI=1S/C17H25NO5/c1-6-13-14(21-4)10-12(8-9-18-11(3)19)16(22-5)17(13)23-15(20)7

InchiKey: UQHVBQZITCKPRN-UHFFFAOYSA-N

Formula: C17H25NO5

SMILES: CCC(=O)Oc1c(CC)c(OC)cc(CCNC(C)=O)c1OC

Mol. weight [g/mol]: 323.38

Physical Properties

Property code	Value	Unit	Source
gf	-317.30	kJ/mol	Joback Method
hf	-771.91	kJ/mol	Joback Method
hfus	44.13	kJ/mol	Joback Method
hvap	85.52	kJ/mol	Joback Method
log10ws	-3.85		Crippen Method
logp	2.260		Crippen Method
mcvol	257.360	ml/mol	McGowan Method
pc	1611.58	kPa	Joback Method
rinpol	2570.00		NIST Webbook
rinpol	2570.00		NIST Webbook
tb	860.13	K	Joback Method
tc	1066.30	K	Joback Method
tf	577.06	K	Joback Method
vc	0.981	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	786.73	J/mol×K	860.13	Joback Method
cpg	800.66	J/mol×K	894.49	Joback Method
cpg	813.42	J/mol×K	928.85	Joback Method
cpg	825.01	J/mol×K	963.22	Joback Method
cpg	835.43	J/mol×K	997.58	Joback Method
cpg	844.64	J/mol×K	1031.94	Joback Method
cpg	852.64	J/mol×K	1066.30	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=R514466&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