4-ethyl-2,5-dimethoxy-«beta»-phenethylamine-M, (hydroxyl-N-acetyl)-isomer 1, acetylated

Inchi: InChI=1S/C16H23NO5/c1-6-12-9-14(20-4)13(7-8-17-10(2)18)16(15(12)21-5)22-11(3)19/h9H,6-8H2,1-5H3,(H,17,18)

InchiKey: FFWYQVFBYRDZPF-UHFFFAOYSA-N

Formula: C16H23NO5

SMILES: CCc1cc(OC)c(CCNC(C)=O)c(OC(C)=O)c1OC

Mol. weight [g/mol]: 309.36

Physical Properties

Property code	Value	Unit	Source
gf	-325.72	kJ/mol	Joback Method
hf	-751.27	kJ/mol	Joback Method
hfus	41.54	kJ/mol	Joback Method
hvap	83.29	kJ/mol	Joback Method
log10ws	-3.43		Crippen Method
logp	1.870		Crippen Method
mcvol	243.270	ml/mol	McGowan Method
pc	1743.37	kPa	Joback Method
rinpol	2340.00		NIST Webbook
tb	837.25	K	Joback Method
tc	1043.33	K	Joback Method
tf	565.79	K	Joback Method
vc	0.924	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	729.35	J/mol×K	837.25	Joback Method
cpg	743.06	J/mol×K	871.60	Joback Method
cpg	755.68	J/mol×K	905.94	Joback Method
cpg	767.19	J/mol×K	940.29	Joback Method
cpg	777.58	J/mol×K	974.64	Joback Method
cpg	786.83	J/mol×K	1008.98	Joback Method
cpg	794.92	J/mol×K	1043.33	Joback Method

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=R514268&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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