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

Inchi: InChI=1S/C15H21NO4/c1-5-12-8-14(19-4)13(6-7-16-10(2)17)9-15(12)20-11(3)18/h8-9H,
InchiKey: WKATUUYRHZTMMY-UHFFFAOYSA-N
Formula: C15H21NO4
SMILES: CCc1cc(OC)c(CCNC(C)=O)cc1OC(C)=O
Mol. weight [g/mol]: 279.33

Physical Properties

Property code	Value	Unit	Source
gf	-219.51	kJ/mol	Joback Method
hf	-586.94	kJ/mol	Joback Method
hfus	38.15	kJ/mol	Joback Method
hvap	77.99	kJ/mol	Joback Method
log10ws	-3.31		Crippen Method
logp	1.861		Crippen Method
mcvol	223.310	ml/mol	McGowan Method
pc	1945.79	kPa	Joback Method
rinpol	2240.00		NIST Webbook
tb	786.97	K	Joback Method
tc	993.33	K	Joback Method
tf	519.77	K	Joback Method
vc	0.851	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	646.71	J/mol×K	786.97	Joback Method
cpg	660.65	J/mol×K	821.36	Joback Method
cpg	673.62	J/mol×K	855.76	Joback Method
cpg	685.62	J/mol×K	890.15	Joback Method
cpg	696.65	J/mol×K	924.55	Joback Method
cpg	706.72	J/mol×K	958.94	Joback Method
cpg	715.82	J/mol×K	993.33	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=R514426&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