4-ethyl-2,5-dimethoxy-«beta»-phenethylamine-M, (O-desmethyl-desamino-COOH), isomer 2, methyl-acetylated

Inchi: InChI=1S/C14H18O5/c1-5-10-6-12(17-8(3)14(15)18-4)7-13(10)19-9(2)15/h6-7H,5,8H2

InchiKey: PMODDNYHBSKUKR-UHFFFAOYSA-N

Formula: C14H18O5

SMILES: CCc1cc(OC)c(CC(=O)OC)cc1OC(C)=O

Mol. weight [g/mol]: 266.29

Physical Properties

Property code	Value	Unit	Source
gf	-422.32	kJ/mol	Joback Method
hf	-751.99	kJ/mol	Joback Method
hfus	31.65	kJ/mol	Joback Method
hvap	71.74	kJ/mol	Joback Method
log10ws	-2.79		Crippen Method
logp	1.898		Crippen Method
mcvol	205.110	ml/mol	McGowan Method
pc	2064.24	kPa	Joback Method
rinpol	2000.00		NIST Webbook
rinpol	2000.00		NIST Webbook
tb	736.34	K	Joback Method
tc	942.40	K	Joback Method
tf	478.07	K	Joback Method
vc	0.777	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	564.66	J/mol×K	736.34	Joback Method
cpg	578.51	J/mol×K	770.68	Joback Method
cpg	591.48	J/mol×K	805.03	Joback Method
cpg	603.54	J/mol×K	839.37	Joback Method
cpg	614.69	J/mol×K	873.71	Joback Method
cpg	624.91	J/mol×K	908.05	Joback Method
cpg	634.16	J/mol×K	942.40	Joback Method
dvisc	0.0005238	Pa×s	478.07	Joback Method

dvisc	0.0003480	Pa×s	521.12	Joback Method
dvisc	0.0002461	Pa×s	564.16	Joback Method
dvisc	0.0001828	Pa×s	607.20	Joback Method
dvisc	0.0001412	Pa×s	650.25	Joback Method
dvisc	0.0001126	Pa×s	693.29	Joback Method
dvisc	0.0000923	Pa×s	736.34	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R514317&Units=SI

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
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