4-iodo-2,5-dimethoxy-«beta»-phenethylamine-M, (desamino-di-HO-O-desmethyl-), triacetylated

Inchi: InChI=1S/C14H15IO6/c1-8(16)19-5-4-11-6-14(21-10(3)18)12(15)7-13(11)20-9(2)17/h6-7
InchiKey: RAPLQXKJQRZHKM-UHFFFAOYSA-N
Formula: C14H15IO6
SMILES: CC(=O)OCCc1cc(OC(C)=O)c(I)cc1OC(C)=O
Mol. weight [g/mol]: 406.17

Physical Properties

Property code	Value	Unit	Source
gf	-493.12	kJ/mol	Joback Method
hf	-787.70	kJ/mol	Joback Method
hfus	37.66	kJ/mol	Joback Method
hvap	87.86	kJ/mol	Joback Method
log10ws	-3.75		Crippen Method
logp	2.247		Crippen Method
mcvol	232.500	ml/mol	McGowan Method
pc	2143.35	kPa	Joback Method
rinpol	2310.00		NIST Webbook
tb	883.35	K	Joback Method
tc	1115.39	K	Joback Method
tf	586.06	K	Joback Method
vc	0.872	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	618.75	J/mol×K	883.35	Joback Method
cpg	628.85	J/mol×K	922.02	Joback Method
cpg	637.79	J/mol×K	960.70	Joback Method
cpg	645.56	J/mol×K	999.37	Joback Method
cpg	652.15	J/mol×K	1038.04	Joback Method
cpg	657.54	J/mol×K	1076.71	Joback Method
cpg	661.71	J/mol×K	1115.39	Joback Method
dvisc	0.0003809	Pa×s	586.06	Joback Method
dvisc	0.0002567	Pa×s	635.61	Joback Method

dvisc	0.0001831	Pa×s	685.16	Joback Method
dvisc	0.0001367	Pa×s	734.71	Joback Method
dvisc	0.0001059	Pa×s	784.25	Joback Method
dvisc	0.0000846	Pa×s	833.80	Joback Method
dvisc	0.0000693	Pa×s	883.35	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=R514520&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