4-iodo-2,5-dimethoxy-«beta»-phenethylamine-M, (desamino-HO-), acetylated

Inchi: InChI=1S/C13H15IO5/c1-8(15)18-5-4-10-6-13(17-3)11(14)7-12(10)19-9(2)16/h6-7H,4-5H

InchiKey: HGOWOSGYCOFNAX-UHFFFAOYSA-N

Formula: C13H15IO5

SMILES: COc1cc(CCOC(C)=O)c(OC(C)=O)cc1I

Mol. weight [g/mol]: 378.16

Physical Properties

Property code	Value	Unit	Source
gf	-372.62	kJ/mol	Joback Method
hf	-654.48	kJ/mol	Joback Method
hfus	33.47	kJ/mol	Joback Method
hvap	78.89	kJ/mol	Joback Method
log10ws	-3.56		Crippen Method
logp	2.331		Crippen Method
mcvol	216.840	ml/mol	McGowan Method
pc	2210.37	kPa	Joback Method
rinpol	2150.00		NIST Webbook
rinpol	2200.00		NIST Webbook
tb	806.60	K	Joback Method
tc	1036.03	K	Joback Method
tf	524.86	K	Joback Method
vc	0.809	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	556.59	J/mol×K	806.60	Joback Method
cpg	568.27	J/mol×K	844.84	Joback Method
cpg	578.93	J/mol×K	883.08	Joback Method
cpg	588.56	J/mol×K	921.32	Joback Method
cpg	597.15	J/mol×K	959.56	Joback Method
cpg	604.67	J/mol×K	997.79	Joback Method
cpg	611.11	J/mol×K	1036.03	Joback Method
dvisc	0.0004750	Pa×s	524.86	Joback Method

dvisc	0.0003149	Pa×s	571.82	Joback Method
dvisc	0.0002221	Pa×s	618.77	Joback Method
dvisc	0.0001646	Pa×s	665.73	Joback Method
dvisc	0.0001269	Pa×s	712.69	Joback Method
dvisc	0.0001011	Pa×s	759.64	Joback Method
dvisc	0.0000826	Pa×s	806.60	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R514535&Units=SI
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

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