4-iodo-2,5-dimethoxy-«beta»-phenethylamine-M, (desamino-HOOC-O-desmethyl-)-H2O

Inchi: InChI=1S/C9H7IO3/c1-12-8-2-5-3-9(11)13-7(5)4-6(8)10/h2-4H,3H2,1H3

InchiKey: VSQWZQYAPBUJCK-UHFFFAOYSA-N

Formula: C9H7IO3

SMILES: COc1cc2c(cc1I)OC(=O)C2

Mol. weight [g/mol]: 290.05

Physical Properties

Property code	Value	Unit	Source
gf	-78.71	kJ/mol	Joback Method
hf	-258.88	kJ/mol	Joback Method
hfus	22.09	kJ/mol	Joback Method
hvap	60.65	kJ/mol	Joback Method
log10ws	-2.91		Crippen Method
logp	1.761		Crippen Method
mcvol	142.180	ml/mol	McGowan Method
pc	3690.97	kPa	Joback Method
rinpol	2080.00		NIST Webbook
rinpol	2080.00		NIST Webbook
tb	668.68	K	Joback Method
tc	938.53	K	Joback Method
tf	452.43	K	Joback Method
vc	0.523	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	312.78	J/mol×K	668.68	Joback Method
cpg	323.78	J/mol×K	713.65	Joback Method
cpg	333.96	J/mol×K	758.63	Joback Method
cpg	343.34	J/mol×K	803.60	Joback Method
cpg	351.94	J/mol×K	848.58	Joback Method
cpg	359.77	J/mol×K	893.55	Joback Method
cpg	366.87	J/mol×K	938.53	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=R514555&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

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