4-iodo-2,5-dimethoxy-«beta»-phenethylamine, deuteromethylene artifact

Inchi: InChI=1S/C11H14INO2/c1-13-5-4-8-6-11(15-3)9(12)7-10(8)14-2/h6-7H,1,4-5H2,2-3H3/i1

InchiKey: WWMQSQLJIYHUGP-DICFDUPASA-N

Formula: C11H12D2INO2

SMILES: C=NCCc1cc(OC)c(I)cc1OC

Mol. weight [g/mol]: 321.15

Physical Properties

Property code	Value	Unit	Source
hf	-165.39	kJ/mol	Joback Method
hvap	61.22	kJ/mol	Joback Method
log10ws	-3.24		Crippen Method
logp	2.551		Crippen Method
mcvol	185.330	ml/mol	McGowan Method
pc	2145.33	kPa	Joback Method
rinpol	1850.00		NIST Webbook
rinpol	1850.00		NIST Webbook
tb	699.88	K	Joback Method
tc	937.91	K	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R514515&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

Legend

hf: Enthalpy of formation 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