

4-iodo-2,5-dimethoxy-«beta»-phenethylamine, methylene 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
InchiKey:	WWMQSQLJIYHUGP-UHFFFAOYSA-N
Formula:	C11H14INO2
SMILES:	C=NCCc1cc(OC)c(I)cc1OC
Mol. weight [g/mol]:	319.14

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	1860.00		NIST Webbook
tb	699.88	K	Joback Method
tc	937.91	K	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=R514604&Units=SI

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

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