N-acetyl-4-Iodo-2,5-dimethoxyphenethylamine

Other names: N-acetyl-2C-I
4-iodo-2,5-dimethoxy-«beta»-phenethylamine, acetylated
Inchi: InChI=1S/C12H16INO3/c1-8(15)14-5-4-9-6-12(17-3)10(13)7-11(9)16-2/h6-7H,4-5H2,1-3H
InchiKey: QRPIDJGCEAORLE-UHFFFAOYSA-N
Formula: C12H16INO3
SMILES: COc1cc(CCN=C(C)O)c(OC)cc1I
Mol. weight [g/mol]: 349.16

Physical Properties

Property code	Value	Unit	Source
hf	-356.26	kJ/mol	Joback Method
hvap	80.83	kJ/mol	Joback Method
log10ws	-3.48		Crippen Method
logp	2.827		Crippen Method
mcvol	205.290	ml/mol	McGowan Method
pc	2167.36	kPa	Joback Method
rinpol	2260.00		NIST Webbook
rinpol	2260.00		NIST Webbook
tb	822.30	K	Joback Method
tc	1046.93	K	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=U379039&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