

# N-acetyl-4-iodo-2,5-dimethoxyphenethylamine

<b>Other names:</b>	N-acetyl-2C-I 4-iodo-2,5-dimethoxy-«beta»-phenethylamine, acetylated
<b>Inchi:</b>	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
<b>InchiKey:</b>	QRPIDJGCEAORLE-UHFFFAOYSA-N
<b>Formula:</b>	C12H16INO3
<b>SMILES:</b>	COc1cc(CCN=C(C)O)c(OC)cc1I
<b>Mol. weight [g/mol]:</b>	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

<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307I">http://pubs.acs.org/doi/abs/10.1021/ci990307I</a>
<b>Crippen Method:</b>	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>
<b>Joback Method:</b>	<a href="https://en.wikipedia.org/wiki/Joback_method">https://en.wikipedia.org/wiki/Joback_method</a>
<b>McGowan Method:</b>	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=U379039&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U379039&amp;Units=SI</a>

## Legend

<b>hf:</b>	Enthalpy of formation at standard conditions
<b>hvac:</b>	Enthalpy of vaporization at standard conditions
<b>log10ws:</b>	Log10 of Water solubility in mol/l
<b>logp:</b>	Octanol/Water partition coefficient
<b>mcvol:</b>	McGowan's characteristic volume
<b>pc:</b>	Critical Pressure
<b>rinqol:</b>	Non-polar retention indices
<b>tb:</b>	Normal Boiling Point Temperature
<b>tc:</b>	Critical Temperature

Latest version available from:

<https://www.cheméo.com/cid/85-392-3/N-acetyl-4-Iodo-2-5-dimethoxyphenethylamine.pdf>

Generated by Cheméo on 2026-06-17 17:03:32.519451021 +0000 UTC m=+5481161.577533243.

Cheméo (<https://www.cheméo.com>) is the biggest free database of chemical and physical data for the process industry.