

# 2C-I

<b>Other names:</b>	4-iodo-2,5-dimethoxy-«beta»-phenethylamine
<b>Inchi:</b>	InChI=1S/C10H14INO2/c1-13-9-6-8(11)10(14-2)5-7(9)3-4-12/h5-6H,3-4,12H2,1-2H3
<b>InchiKey:</b>	PQHQB RJAAZQXHL-UHFFFAOYSA-N
<b>Formula:</b>	C10H14INO2
<b>SMILES:</b>	<chem>COc1cc(CCN)c(OC)cc1I</chem>
<b>Mol. weight [g/mol]:</b>	307.13
<b>CAS:</b>	64584-32-3

## Physical Properties

Property code	Value	Unit	Source
gf	31.41	kJ/mol	Joback Method
hf	-201.39	kJ/mol	Joback Method
hfus	26.51	kJ/mol	Joback Method
hvap	66.95	kJ/mol	Joback Method
log10ws	-3.10		Crippen Method
logp	1.810		Crippen Method
mcvol	175.540	ml/mol	McGowan Method
pc	2796.51	kPa	Joback Method
rinpol	2330.00		NIST Webbook
rinpol	2330.00		NIST Webbook
tb	680.33	K	Joback Method
tc	920.10	K	Joback Method
tf	452.22	K	Joback Method
vc	0.640	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	411.26	J/mol×K	680.33	Joback Method
cpg	423.90	J/mol×K	720.29	Joback Method
cpg	435.74	J/mol×K	760.25	Joback Method
cpg	446.76	J/mol×K	800.21	Joback Method
cpg	456.97	J/mol×K	840.17	Joback Method
cpg	466.38	J/mol×K	880.14	Joback Method

## Sources

<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=C64584323&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C64584323&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</a>

## Legend

<b>cpg:</b>	Ideal gas heat capacity
<b>gf:</b>	Standard Gibbs free energy of formation
<b>hf:</b>	Enthalpy of formation at standard conditions
<b>hfus:</b>	Enthalpy of fusion at standard conditions
<b>hvap:</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>rinpol:</b>	Non-polar retention indices
<b>tb:</b>	Normal Boiling Point Temperature
<b>tc:</b>	Critical Temperature
<b>tf:</b>	Normal melting (fusion) point
<b>vc:</b>	Critical Volume

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