4-iodo-2,5-dimethoxy-«beta»-phenethylamine-M, (O-desmethyl-N-acetyl-), isomer-2

Inchi: InChI=1S/C11H14INO3/c1-7(14)13-4-3-8-5-10(15)9(12)6-11(8)16-2/h5-6,15H,3-4H2,1-2H

InchiKey: DGSCQLFXCHSXPE-UHFFFAOYSA-N

Formula: C11H14INO3

SMILES: COc1cc(I)c(O)cc1CCNC(C)=O

Mol. weight [g/mol]: 335.14

Physical Properties

Property code	Value	Unit	Source
gf	-106.14	kJ/mol	Joback Method
hf	-348.55	kJ/mol	Joback Method
hfus	35.58	kJ/mol	Joback Method
hvap	81.66	kJ/mol	Joback Method
log10ws	-2.89		Crippen Method
logp	1.684		Crippen Method
mcvol	191.200	ml/mol	McGowan Method
pc	3131.49	kPa	Joback Method
rinpol	2520.00		NIST Webbook
rinpol	2520.00		NIST Webbook
tb	787.94	K	Joback Method
tc	1030.10	K	Joback Method
tf	559.79	K	Joback Method
vc	0.656	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	486.21	J/mol×K	787.94	Joback Method
cpg	497.26	J/mol×K	828.30	Joback Method
cpg	507.67	J/mol×K	868.66	Joback Method
cpg	517.54	J/mol×K	909.02	Joback Method
cpg	526.95	J/mol×K	949.38	Joback Method
cpg	535.98	J/mol×K	989.74	Joback Method
cpg	544.71	J/mol×K	1030.10	Joback Method

Sources

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=R514664&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion 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
tf:	Normal melting (fusion) point
vc:	Critical Volume