4-iodo-2,5-dimethoxy-«beta»-phenethylamine-M, (O-desmethyl-), isomer 1, diacetylated

Inchi: InChI=1S/C13H16INO4/c1-8(16)15-5-4-10-6-13(18-3)11(14)7-12(10)19-9(2)17/h6-7H,4-5

InchiKey: PXRNCMNJWCNTKT-UHFFFAOYSA-N

Formula: C13H16INO4

SMILES: COc1cc(CCNC(C)=O)c(OC(C)=O)cc1I

Mol. weight [g/mol]: 377.17

Physical Properties

Property code	Value	Unit	Source
gf	-178.23	kJ/mol	Joback Method
hf	-468.79	kJ/mol	Joback Method
hfus	37.38	kJ/mol	Joback Method
hvap	82.91	kJ/mol	Joback Method
log10ws	-3.66		Crippen Method
logp	1.904		Crippen Method
mcvol	220.950	ml/mol	McGowan Method
pc	2274.07	kPa	Joback Method
rinpol	2480.00		NIST Webbook
rinpol	2480.00		NIST Webbook
tb	834.35	K	Joback Method
tc	1065.10	K	Joback Method
tf	555.29	K	Joback Method
vc	0.827	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	581.59	J/mol×K	834.35	Joback Method
cpg	592.96	J/mol×K	872.81	Joback Method
cpg	603.33	J/mol×K	911.27	Joback Method
cpg	612.71	J/mol×K	949.72	Joback Method
cpg	621.09	J/mol×K	988.18	Joback Method
cpg	628.48	J/mol×K	1026.64	Joback Method
cpg	634.89	J/mol×K	1065.10	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=R514619&Units=SI

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