4-iodo-2,5-dimethoxy-«beta»-phenethylamine-M, (desamino-HOOC-), methyl

Inchi: InChI=1S/C11H13IO4/c1-14-9-6-8(12)10(15-2)4-7(9)5-11(13)16-3/h4,6H,5H2,1-3H3
InchiKey: WHHDCUHNLUQVAM-UHFFFAOYSA-N
Formula: C11H13IO4
SMILES: COC(=O)Cc1cc(OC)c(I)cc1OC
Mol. weight [g/mol]: 336.12

Physical Properties

Property code	Value	Unit	Source
gf	-260.54	kJ/mol	Joback Method
hf	-500.62	kJ/mol	Joback Method
hfus	26.69	kJ/mol	Joback Method
hvap	67.69	kJ/mol	Joback Method
log10ws	-2.94		Crippen Method
logp	2.024		Crippen Method
mcvol	187.090	ml/mol	McGowan Method
pc	2505.01	kPa	Joback Method
rinpol	2115.00		NIST Webbook
tb	706.97	K	Joback Method
tc	938.81	K	Joback Method
tf	452.39	K	Joback Method
vc	0.692	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	441.27	J/mol×K	706.97	Joback Method
cpg	453.55	J/mol×K	745.61	Joback Method
cpg	465.01	J/mol×K	784.25	Joback Method
cpg	475.63	J/mol×K	822.89	Joback Method
cpg	485.38	J/mol×K	861.53	Joback Method
cpg	494.24	J/mol×K	900.17	Joback Method
cpg	502.19	J/mol×K	938.81	Joback Method
dvisc	0.0006240	Pa×s	452.39	Joback Method
dvisc	0.0004117	Pa×s	494.82	Joback Method

dvisc	0.0002901	Pa×s	537.25	Joback Method
dvisc	0.0002152	Pa×s	579.68	Joback Method
dvisc	0.0001662	Pa×s	622.11	Joback Method
dvisc	0.0001327	Pa×s	664.54	Joback Method
dvisc	0.0001089	Pa×s	706.97	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=R514540&Units=SI

Legend

cpg: Ideal gas heat capacity
dvisc: Dynamic viscosity
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