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

Inchi: InChI=1S/C12H10F3IO5/c1-19-9-3-6(4-10(17)20-2)8(5-7(9)16)21-11(18)12(13,14)15/h3,5
InchiKey: IGHFFEJPFCMPCJ-UHFFFAOYSA-N
Formula: C12H10F3IO5
SMILES: COC(=O)Cc1cc(OC)c(I)cc1OC(=O)C(F)(F)F
Mol. weight [g/mol]: 418.10

Physical Properties

Property code	Value	Unit	Source
gf	-962.63	kJ/mol	Joback Method
hf	-1230.92	kJ/mol	Joback Method
hfus	32.70	kJ/mol	Joback Method
hvap	72.92	kJ/mol	Joback Method
log10ws	-3.80		Crippen Method
logp	2.483		Crippen Method
mcvol	208.060	ml/mol	McGowan Method
pc	2169.38	kPa	Joback Method
rinpol	1980.00		NIST Webbook
rinpol	1980.00		NIST Webbook
tb	778.30	K	Joback Method
tc	996.24	K	Joback Method
tf	517.78	K	Joback Method
vc	0.796	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	528.81	J/mol×K	778.30	Joback Method
cpg	538.70	J/mol×K	814.62	Joback Method
cpg	547.75	J/mol×K	850.95	Joback Method
cpg	555.96	J/mol×K	887.27	Joback Method
cpg	563.33	J/mol×K	923.59	Joback Method
cpg	569.88	J/mol×K	959.92	Joback Method
cpg	575.61	J/mol×K	996.24	Joback Method

Sources

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=R514560&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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