4-iodo-2,5-dimethoxy-«beta»-phenethylamine, TFA

Inchi: InChI=1S/C12H13F3INO3/c1-19-9-6-8(16)10(20-2)5-7(9)3-4-17-11(18)12(13,14)15/h5-6H

InchiKey: ANNXCJDPSSBHSR-UHFFFAOYSA-N

Formula: C12H13F3INO3

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

Mol. weight [g/mol]: 403.14

Physical Properties

Property code	Value	Unit	Source
gf	-639.32	kJ/mol	Joback Method
hf	-932.65	kJ/mol	Joback Method
hfus	35.02	kJ/mol	Joback Method
hvap	70.20	kJ/mol	Joback Method
log10ws	-4.13		Crippen Method
logp	2.529		Crippen Method
mcvol	210.600	ml/mol	McGowan Method
pc	2104.20	kPa	Joback Method
rinpol	2100.00		NIST Webbook
tb	752.18	K	Joback Method
tc	965.84	K	Joback Method
tf	498.28	K	Joback Method
vc	0.807	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	543.77	J/mol×K	752.18	Joback Method
cpg	554.98	J/mol×K	787.79	Joback Method
cpg	565.35	J/mol×K	823.40	Joback Method
cpg	574.93	J/mol×K	859.01	Joback Method
cpg	583.73	J/mol×K	894.62	Joback Method
cpg	591.79	J/mol×K	930.23	Joback Method
cpg	599.13	J/mol×K	965.84	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=R514679&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