2,5-Dimethoxy-4-methyl-«beta»-phenethylamine-N (O-desmethyl), bisTFA,I

Inchi: InChI=1S/C14H13F6NO4/c1-7-5-10(25-12(23)14(18,19)20)8(6-9(7)24-2)3-4-21-11(22)13

InchiKey: PSRUCKTBFMYIM-UHFFFAOYSA-N

Formula: C14H13F6NO4

SMILES: COc1cc(CCNC(=O)C(F)(F)F)c(OC(=O)C(F)(F)F)cc1C

Mol. weight [g/mol]: 373.25

Physical Properties

Property code	Value	Unit	Source
gf	-1391.11	kJ/mol	Joback Method
hf	-1760.46	kJ/mol	Joback Method
hfus	39.21	kJ/mol	Joback Method
hvap	68.27	kJ/mol	Joback Method
log10ws	-4.31		Crippen Method
logp	2.692		Crippen Method
mcvol	219.840	ml/mol	McGowan Method
pc	1731.78	kPa	Joback Method
rinpol	1780.00		NIST Webbook
rinpol	1780.00		NIST Webbook
tb	753.25	K	Joback Method
tc	939.82	K	Joback Method
tf	516.88	K	Joback Method
vc	0.880	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	642.68	J/mol×K	753.25	Joback Method
cpg	653.85	J/mol×K	784.35	Joback Method
cpg	664.23	J/mol×K	815.44	Joback Method
cpg	673.85	J/mol×K	846.54	Joback Method
cpg	682.74	J/mol×K	877.63	Joback Method
cpg	690.93	J/mol×K	908.73	Joback Method
cpg	698.46	J/mol×K	939.82	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R438298&Units=SI
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

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