4-ethyl-2,5-dimethoxy-«beta»-phenethylamine-M, (O-desmethyl), isomer 2, 2TFA

Inchi: InChI=1S/C15H15F6NO4/c1-3-8-6-10(25-2)9(4-5-22-12(23)14(16,17)18)7-11(8)26-13(24
InchiKey: GFHBXMUAOKRMRE-UHFFFAOYSA-N
Formula: C15H15F6NO4
SMILES: CCc1cc(OC)c(CCNC(=O)C(F)(F)F)cc1OC(=O)C(F)(F)F
Mol. weight [g/mol]: 387.27

Physical Properties

Property code	Value	Unit	Source
gf	-1382.69	kJ/mol	Joback Method
hf	-1781.10	kJ/mol	Joback Method
hfus	41.80	kJ/mol	Joback Method
hvap	70.50	kJ/mol	Joback Method
log10ws	-4.64		Crippen Method
logp	2.946		Crippen Method
mcvol	233.930	ml/mol	McGowan Method
pc	1601.28	kPa	Joback Method
rinpol	1810.00		NIST Webbook
rinpol	1810.00		NIST Webbook
tb	776.13	K	Joback Method
tc	963.18	K	Joback Method
tf	528.15	K	Joback Method
vc	0.936	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	696.59	J/mol×K	776.13	Joback Method
cpg	708.18	J/mol×K	807.30	Joback Method
cpg	718.94	J/mol×K	838.48	Joback Method
cpg	728.92	J/mol×K	869.65	Joback Method
cpg	738.14	J/mol×K	900.83	Joback Method
cpg	746.64	J/mol×K	932.00	Joback Method
cpg	754.45	J/mol×K	963.18	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R514406&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