2,5-Dimethoxy-4-methyl-«beta»-phenethylamine-M (HO-), bisTFA

Inchi: InChI=1S/C15H14F6O6/c1-7-9(24-2)6-8(4-5-26-12(22)14(16,17)18)11(25-3)10(7)27-13(2
InchiKey: NZFZZPYLUZXZDE-UHFFFAOYSA-N
Formula: C15H14F6O6
SMILES: COc1cc(CCOC(=O)C(F)(F)F)c(OC)c(OC(=O)C(F)(F)F)c1C
Mol. weight [g/mol]: 404.26

Physical Properties

Property code	Value	Unit	Source
gf	-1691.71	kJ/mol	Joback Method
hf	-2110.48	kJ/mol	Joback Method
hfus	38.69	kJ/mol	Joback Method
hvap	69.55	kJ/mol	Joback Method
log10ws	-4.33		Crippen Method
logp	3.128		Crippen Method
mcvol	235.690	ml/mol	McGowan Method
pc	1524.69	kPa	Joback Method
rinpol	1950.00		NIST Webbook
tb	775.78	K	Joback Method
tc	961.43	K	Joback Method
tf	532.47	K	Joback Method
vc	0.938	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	695.16	J/mol×K	775.78	Joback Method
cpg	706.66	J/mol×K	806.72	Joback Method
cpg	717.33	J/mol×K	837.66	Joback Method
cpg	727.18	J/mol×K	868.60	Joback Method
cpg	736.20	J/mol×K	899.54	Joback Method
cpg	744.41	J/mol×K	930.48	Joback Method
cpg	751.80	J/mol×K	961.43	Joback Method

Sources

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=R438283&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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