4-ethyl-2,5-dimethoxy-«beta»-phenethylamine-M, (HO-), 2TFA

InChI: InChI=1S/C16H17F6NO5/c1-4-9-10(26-2)7-8(5-6-23-13(24)15(17,18)19)11(27-3)12(9)28
InChIKey: BVPRNYOFSCTSPO-UHFFFAOYSA-N
Formula: C16H17F6NO5
SMILES: CCc1c(OC)cc(CCNC(=O)C(F)(F)F)c(OC)c1OC(=O)C(F)(F)F
Mol. weight [g/mol]: 417.30

Physical Properties

Property code	Value	Unit	Source
gf	-1488.90	kJ/mol	Joback Method
hf	-1945.43	kJ/mol	Joback Method
hfus	45.19	kJ/mol	Joback Method
hvap	75.80	kJ/mol	Joback Method
log10ws	-4.76		Crippen Method
logp	2.955		Crippen Method
mcvol	253.890	ml/mol	McGowan Method
pc	1449.04	kPa	Joback Method
rinpol	2040.00		NIST Webbook
tb	826.41	K	Joback Method
tc	1017.50	K	Joback Method
tf	574.17	K	Joback Method
vc	1.010	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	777.06	J/mol×K	826.41	Joback Method
cpg	788.71	J/mol×K	858.26	Joback Method
cpg	799.45	J/mol×K	890.11	Joback Method
cpg	809.31	J/mol×K	921.96	Joback Method
cpg	818.31	J/mol×K	953.80	Joback Method
cpg	826.47	J/mol×K	985.65	Joback Method
cpg	833.82	J/mol×K	1017.50	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=R514213&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