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

Inchi: InChI=1S/C16H20F3NO5/c1-5-10-8-12(23-3)11(6-7-20-9(2)21)14(13(10)24-4)25-15(22)1

InchiKey: PPYDCOINDOERST-UHFFFAOYSA-N

Formula: C16H20F3NO5

SMILES: CCc1cc(OC)c(CCNC(C)=O)c(OC(=O)C(F)(F)F)c1OC

Mol. weight [g/mol]: 363.33

Physical Properties

Property code	Value	Unit	Source
gf	-907.31	kJ/mol	Joback Method
hf	-1348.35	kJ/mol	Joback Method
hfus	43.37	kJ/mol	Joback Method
hvap	79.55	kJ/mol	Joback Method
log10ws	-4.09		Crippen Method
logp	2.412		Crippen Method
mcvol	248.580	ml/mol	McGowan Method
pc	1586.01	kPa	Joback Method
rinpol	2080.00		NIST Webbook
tb	831.83	K	Joback Method
tc	1029.48	K	Joback Method
tf	569.98	K	Joback Method
vc	0.968	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	753.10	J/mol×K	831.83	Joback Method
cpg	765.70	J/mol×K	864.77	Joback Method
cpg	777.32	J/mol×K	897.71	Joback Method
cpg	787.97	J/mol×K	930.66	Joback Method
cpg	797.64	J/mol×K	963.60	Joback Method
cpg	806.34	J/mol×K	996.54	Joback Method
cpg	814.09	J/mol×K	1029.48	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=R514248&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

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