Benzeneethanamine, 3,4-dimethoxy-N-[(pentafluorophenyl)methylene]-

Other names: 2-(3,4-Dimethoxyphenyl)ethylamine, PFB-imine
Inchi: InChI=1S/C17H14F5NO2/c1-24-11-4-3-9(7-12(11)25-2)5-6-23-8-10-13(18)15(20)17(22)1
InchiKey: OVZBSJFTHDKGIV-UHFFFAOYSA-N
Formula: C17H14F5NO2
SMILES: COc1ccc(CCN=Cc2c(F)c(F)c(F)c(F)c2F)cc1OC
Mol. weight [g/mol]: 359.29
CAS: 55334-05-9

Physical Properties

Property code	Value	Unit	Source
hf	-1164.21	kJ/mol	Joback Method
hvap	66.67	kJ/mol	Joback Method
log10ws	-5.47		Crippen Method
logp	4.061		Crippen Method
mcvol	229.140	ml/mol	McGowan Method
pc	1416.50	kPa	Joback Method
rinpol	2075.00		NIST Webbook
rinpol	2075.00		NIST Webbook
tb	794.45	K	Joback Method
tc	995.06	K	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C55334059&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
McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Legend

hf:	Enthalpy of formation 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