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

Inchi: InChI=1S/C15H16F3NO5/c1-8(20)11-7-12(23-3)10(4-5-19-9(2)21)6-13(11)24-14(22)15(1

InchiKey: ZGXQPGGIZHJZQD-UHFFFAOYSA-N

Formula: C15H16F3NO5

SMILES: COc1cc(C(C)=O)c(OC(=O)C(F)(F)F)cc1CCNC(C)=O

Mol. weight [g/mol]: 347.29

Physical Properties

Property code	Value	Unit	Source
gf	-930.02	kJ/mol	Joback Method
hf	-1296.60	kJ/mol	Joback Method
hfus	41.58	kJ/mol	Joback Method
hvap	80.99	kJ/mol	Joback Method
log10ws	-3.83		Crippen Method
logp	2.044		Crippen Method
mcvol	230.190	ml/mol	McGowan Method
pc	1857.91	kPa	Joback Method
rinpol	2120.00		NIST Webbook
tb	835.42	K	Joback Method
tc	1038.65	K	Joback Method
tf	573.89	K	Joback Method
vc	0.899	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	683.74	J/mol×K	835.42	Joback Method
cpg	694.84	J/mol×K	869.29	Joback Method
cpg	705.02	J/mol×K	903.16	Joback Method
cpg	714.29	J/mol×K	937.04	Joback Method
cpg	722.67	J/mol×K	970.91	Joback Method
cpg	730.18	J/mol×K	1004.78	Joback Method
cpg	736.84	J/mol×K	1038.65	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=R514446&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