2,5-Dimethoxy-4-methyl-«beta»-phenethylamine-N (O-desmethyl-N-acetyl-), TFA, T

Inchi: InChI=1S/C14H16F3NO4/c1-8-6-12(22-13(20)14(15,16)17)10(7-11(8)21-3)4-5-18-9(2)19

InchiKey: RUAIOXFTYGEUNP-UHFFFAOYSA-N

Formula: C14H16F3NO4

SMILES: COc1cc(CCNC(C)=O)c(OC(=O)C(F)(F)F)cc1C

Mol. weight [g/mol]: 319.28

Physical Properties

Property code	Value	Unit	Source
gf	-809.52	kJ/mol	Joback Method
hf	-1163.38	kJ/mol	Joback Method
hfus	37.39	kJ/mol	Joback Method
hvap	72.02	kJ/mol	Joback Method
log10ws	-3.65		Crippen Method
logp	2.150		Crippen Method
mcvol	214.530	ml/mol	McGowan Method
pc	1911.91	kPa	Joback Method
rinpol	1990.00		NIST Webbook
rinpol	1990.00		NIST Webbook
tb	758.67	K	Joback Method
tc	955.03	K	Joback Method
tf	512.69	K	Joback Method
vc	0.838	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	617.07	J/mol×K	758.67	Joback Method
cpg	629.36	J/mol×K	791.40	Joback Method
cpg	640.81	J/mol×K	824.12	Joback Method
cpg	651.42	J/mol×K	856.85	Joback Method
cpg	661.23	J/mol×K	889.57	Joback Method
cpg	670.25	J/mol×K	922.30	Joback Method
cpg	678.48	J/mol×K	955.03	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=R438352&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