Phenethylamine, 2,5-dimethoxy-4-propylthio, N-acetyl, trifluoroacetoxy-M

Inchi: InChI=1S/C17H22F3NO5S/c1-5-8-27-15-12(24-3)9-11(6-7-21-10(2)22)13(25-4)14(15)26

InchiKey: FQGPLPUEGZRAJX-UHFFFAOYSA-N

Formula: C17H22F3NO5S

SMILES: CCCSc1c(OC)cc(CCNC(C)=O)c(OC)c1OC(=O)C(F)(F)F

Mol. weight [g/mol]: 409.42

Physical Properties

Property code	Value	Unit	Source
gf	-865.77	kJ/mol	Joback Method
hf	-1327.12	kJ/mol	Joback Method
hfus	50.09	kJ/mol	Joback Method
hvap	88.59	kJ/mol	Joback Method
log10ws	-4.87		Crippen Method
logp	3.352		Crippen Method
mcvol	279.020	ml/mol	McGowan Method
pc	1490.74	kPa	Joback Method
rinpol	2350.00		NIST Webbook
rinpol	2350.00		NIST Webbook
tb	923.49	K	Joback Method
tc	1136.13	K	Joback Method
tf	615.65	K	Joback Method
vc	1.077	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	862.50	J/mol×K	923.49	Joback Method
cpg	873.84	J/mol×K	958.93	Joback Method
cpg	883.90	J/mol×K	994.37	Joback Method
cpg	892.70	J/mol×K	1029.81	Joback Method
cpg	900.23	J/mol×K	1065.25	Joback Method
cpg	906.50	J/mol×K	1100.69	Joback Method
cpg	911.50	J/mol×K	1136.13	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=R418625&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