Phenethylamine, 2,5-dimethoxy-4-propylthio, N-acetyl, sulfone, acetoxy-M

Inchi: InChI=1S/C17H25NO7S/c1-6-9-26(21,22)17-14(23-4)10-13(7-8-18-11(2)19)15(24-5)16(1

InchiKey: XKTSEIISPXQCTI-UHFFFAOYSA-N

Formula: C17H25NO7S

SMILES: CCCS(=O)(=O)c1c(OC)cc(CCN=C(C)O)c(OC)c1OC(C)=O

Mol. weight [g/mol]: 387.45

Physical Properties

Property code	Value	Unit	Source
hf	-1245.95	kJ/mol	Joback Method
hvap	111.04	kJ/mol	Joback Method
log10ws	-3.18		Crippen Method
logp	2.332		Crippen Method
mcvol	285.450	ml/mol	McGowan Method
pc	1707.53	kPa	Joback Method
rinpol	2760.00		NIST Webbook
rinpol	2760.00		NIST Webbook
tb	972.61	K	Joback Method
tc	1191.14	K	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R418610&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