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

Inchi: InChI=1S/C15H23NO4S/c1-5-8-21-15-12(19-3)9-11(6-7-16-10(2)17)14(20-4)13(15)18/h9

InchiKey: XGTRKCZLXMGTQQ-UHFFFAOYSA-N

Formula: C15H23NO4S

SMILES: CCCSc1c(OC)cc(CCN=C(C)O)c(OC)c1O

Mol. weight [g/mol]: 313.41

Physical Properties

Property code	Value	Unit	Source
hf	-630.49	kJ/mol	Joback Method
hvap	97.97	kJ/mol	Joback Method
log10ws	-3.46		Crippen Method
logp	3.430		Crippen Method
mcvol	243.960	ml/mol	McGowan Method
pc	1978.82	kPa	Joback Method
rinpol	2740.00		NIST Webbook
rinpol	2740.00		NIST Webbook
tb	947.20	K	Joback Method
tc	1171.25	K	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R418605&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

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