Phenethylamine, 2,5-dimethoxy-4-propylthio, N-methylene

Inchi: InChI=1S/C14H21NO2S/c1-5-8-18-14-10-12(16-3)11(6-7-15-2)9-13(14)17-4/h9-10H,2,5-

InchiKey: IMGMLSCTAZSZBT-UHFFFAOYSA-N

Formula: C14H21NO2S

SMILES: C=NCCc1cc(OC)c(SCCC)cc1OC

Mol. weight [g/mol]: 267.39

Physical Properties

Property code	Value	Unit	Source
hf	-262.31	kJ/mol	Joback Method
hvap	65.34	kJ/mol	Joback Method
log10ws	-3.68		Crippen Method
logp	3.449		Crippen Method
mcvol	218.130	ml/mol	McGowan Method
pc	1724.59	kPa	Joback Method
rinpol	2060.00		NIST Webbook
rinpol	2060.00		NIST Webbook
tb	744.16	K	Joback Method
tc	962.38	K	Joback Method

Sources

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=R418630&Units=SI

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

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