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

Inchi: InChI=1S/C17H25NO5S/c1-6-9-24-17-14(21-4)10-13(7-8-18-11(2)19)15(22-5)16(17)23-1

InchiKey: GUSMHIMYTGDYGX-UHFFFAOYSA-N

Formula: C17H25NO5S

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

Mol. weight [g/mol]: 355.45

Physical Properties

Property code	Value	Unit	Source
gf	-284.18	kJ/mol	Joback Method
hf	-730.04	kJ/mol	Joback Method
hfus	48.26	kJ/mol	Joback Method
hvap	92.33	kJ/mol	Joback Method
log10ws	-4.21		Crippen Method
logp	2.810		Crippen Method
mcvol	273.710	ml/mol	McGowan Method
pc	1633.81	kPa	Joback Method
rinpol	2590.00		NIST Webbook
tb	928.91	K	Joback Method
tc	1148.36	K	Joback Method
tf	611.46	K	Joback Method
vc	1.034	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	840.39	J/mol×K	928.91	Joback Method
cpg	852.55	J/mol×K	965.48	Joback Method
cpg	863.27	J/mol×K	1002.06	Joback Method
cpg	872.51	J/mol×K	1038.63	Joback Method
cpg	880.25	J/mol×K	1075.21	Joback Method
cpg	886.48	J/mol×K	1111.78	Joback Method
cpg	891.16	J/mol×K	1148.36	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=R418596&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