Phenethylamine, 2,5-dimethoxy-4-mercapto, N-acetyl

Inchi: InChI=1S/C12H17NO3S/c1-8(14)13-5-4-9-6-11(16-3)12(17)7-10(9)15-2/h6-7,17H,4-5H2,

InchiKey: PPQHFWLKYPAVPB-UHFFFAOYSA-N

Formula: C12H17NO3S

SMILES: COc1cc(CCNC(C)=O)c(OC)cc1S

Mol. weight [g/mol]: 255.33

Physical Properties

Property code	Value	Unit	Source
gf	-86.46	kJ/mol	Joback Method
hf	-373.96	kJ/mol	Joback Method
hfus	32.83	kJ/mol	Joback Method
hvap	71.31	kJ/mol	Joback Method
log10ws	-2.83		Crippen Method
logp	1.671		Crippen Method
mcvol	195.820	ml/mol	McGowan Method
pc	2555.92	kPa	Joback Method
rinpol	2170.00		NIST Webbook
tb	727.32	K	Joback Method
tc	949.06	K	Joback Method
tf	472.49	K	Joback Method
vc	0.731	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	519.90	J/mol×K	727.32	Joback Method
cpg	533.59	J/mol×K	764.28	Joback Method
cpg	546.36	J/mol×K	801.23	Joback Method
cpg	558.20	J/mol×K	838.19	Joback Method
cpg	569.12	J/mol×K	875.14	Joback Method
cpg	579.10	J/mol×K	912.10	Joback Method
cpg	588.14	J/mol×K	949.06	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=R418536&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