Phenethylamine, 2,5-dimethoxy-4-methylthio, sulfoxide, N-acetyl

Inchi: InChI=1S/C13H19NO4S/c1-9(15)14-6-5-10-7-12(18-3)13(19(4)16)8-11(10)17-2/h7-8H,5-

InchiKey: MMLNTVMTTLMSNV-UHFFFAOYSA-N

Formula: C13H19NO4S

SMILES: COc1cc(S(C)=O)c(OC)cc1CCNC(C)=O

Mol. weight [g/mol]: 285.36

Physical Properties

Property code	Value	Unit	Source
gf	-325.14	kJ/mol	Joback Method
hf	-638.82	kJ/mol	Joback Method
hfus	39.13	kJ/mol	Joback Method
hvap	79.52	kJ/mol	Joback Method
log10ws	-1.81		Crippen Method
logp	1.120		Crippen Method
mcvol	215.780	ml/mol	McGowan Method
pc	2374.90	kPa	Joback Method
rinpol	2460.00		NIST Webbook
rinpol	2460.00		NIST Webbook
tb	745.62	K	Joback Method
tc	953.86	K	Joback Method
tf	483.78	K	Joback Method
vc	0.823	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	593.75	J/mol×K	745.62	Joback Method
cpg	607.77	J/mol×K	780.33	Joback Method
cpg	620.82	J/mol×K	815.03	Joback Method
cpg	632.87	J/mol×K	849.74	Joback Method
cpg	643.91	J/mol×K	884.45	Joback Method
cpg	653.92	J/mol×K	919.15	Joback Method
cpg	662.89	J/mol×K	953.86	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R418561&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

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