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

Inchi: InChI=1S/C13H19NO5S/c1-9(15)14-6-5-10-7-12(19-3)13(20(4,16)17)8-11(10)18-2/h7-8H

InchiKey: OSUXFKASJLCWDW-UHFFFAOYSA-N

Formula: C13H19NO5S

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

Mol. weight [g/mol]: 301.36

Physical Properties

Property code	Value	Unit	Source
gf	-575.97	kJ/mol	Joback Method
hf	-886.43	kJ/mol	Joback Method
hfus	42.75	kJ/mol	Joback Method
hvap	85.43	kJ/mol	Joback Method
log10ws	-2.01		Crippen Method
logp	0.786		Crippen Method
mcvol	221.650	ml/mol	McGowan Method
pc	2543.05	kPa	Joback Method
rinpol	2580.00		NIST Webbook
rinpol	2580.00		NIST Webbook
tb	735.12	K	Joback Method
tc	934.27	K	Joback Method
tf	485.86	K	Joback Method
vc	0.859	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	610.34	J/mol×K	735.12	Joback Method
cpg	624.33	J/mol×K	768.31	Joback Method
cpg	637.37	J/mol×K	801.50	Joback Method
cpg	649.44	J/mol×K	834.69	Joback Method
cpg	660.53	J/mol×K	867.88	Joback Method
cpg	670.60	J/mol×K	901.07	Joback Method
cpg	679.66	J/mol×K	934.27	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R418556&Units=SI

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