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

**Inchi:** InChI=1S/C13H19NO3S/c1-9(15)14-6-5-10-7-12(17-3)13(18-4)8-11(10)16-2/h7-8H,5-6H
**InchiKey:** IXIKVQQQZVKSLD-UHFFFAOYSA-N
**Formula:** C13H19NO3S
**SMILES:** COc1cc(SC)c(OC)cc1CCNC(C)=O
**Mol. weight [g/mol]:** 269.36

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -74.31 | kJ/mol | Joback Method |
| hf | -391.21 | kJ/mol | Joback Method |
| hfus | 35.50 | kJ/mol | Joback Method |
| hvap | 73.61 | kJ/mol | Joback Method |
| log10ws | -3.06 | | Crippen Method |
| logp | 2.104 | | Crippen Method |
| mcvol | 209.910 | ml/mol | McGowan Method |
| pc | 2222.89 | kPa | Joback Method |
| rinpol | 2230.00 | | NIST Webbook |
| rinpol | 2230.00 | | NIST Webbook |
| tb | 756.12 | K | Joback Method |
| tc | 974.23 | K | Joback Method |
| tf | 481.70 | K | Joback Method |
| vc | 0.786 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 576.89 | J/mol×K | 756.12 | Joback Method |
| cpg | 590.98 | J/mol×K | 792.47 | Joback Method |
| cpg | 604.07 | J/mol×K | 828.82 | Joback Method |
| cpg | 616.15 | J/mol×K | 865.17 | Joback Method |
| cpg | 627.19 | J/mol×K | 901.52 | Joback Method |
| cpg | 637.20 | J/mol×K | 937.88 | Joback Method |
| cpg | 646.16 | J/mol×K | 974.23 | Joback Method |

# Sources

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|---|---|
| **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=R418541&Units=SI |

# Legend

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|---|---|
| **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 |