

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

| | |
|----------------------|---|
| Inchi: | InChI=1S/C17H25NO7S/c1-6-9-26(21,22)17-14(23-4)10-13(7-8-18-11(2)19)15(24-5)16(1) |
| InchiKey: | XKTSEIISPXQCTI-UHFFFAOYSA-N |
| Formula: | C17H25NO7S |
| SMILES: | CCCS(=O)(=O)c1c(OC)cc(CCN=C(C)O)c(OC)c1OC(C)=O |
| Mol. weight [g/mol]: | 387.45 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|----------|--------|----------------|
| hf | -1245.95 | kJ/mol | Joback Method |
| hvap | 111.04 | kJ/mol | Joback Method |
| log10ws | -3.18 | | Crippen Method |
| logp | 2.332 | | Crippen Method |
| mcvol | 285.450 | ml/mol | McGowan Method |
| pc | 1707.53 | kPa | Joback Method |
| rinpol | 2760.00 | | NIST Webbook |
| rinpol | 2760.00 | | NIST Webbook |
| tb | 972.61 | K | Joback Method |
| tc | 1191.14 | K | 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=R418610&Units=SI |
| Crippen Method: | http://pubs.acs.org/doi/abs/10.1021/ci990307l |

Legend

| | |
|-------|---|
| hf: | Enthalpy of formation at standard conditions |
| hvap: | Enthalpy of vaporization at standard conditions |

| | |
|-----------------|-------------------------------------|
| log10ws: | Log10 of Water solubility in mol/l |
| logp: | Octanol/Water partition coefficient |
| mvol: | McGowan's characteristic volume |
| pc: | Critical Pressure |
| rinpol: | Non-polar retention indices |
| tb: | Normal Boiling Point Temperature |
| tc: | Critical Temperature |

Latest version available from:

<https://www.chemeo.com/cid/90-462-9/Phenethylamine-2-5-dimethoxy-4-propylthio-N-acetyl-sulfone-acetoxy-M.pdf>

Generated by Cheméo on 2024-04-10 18:52:22.807738373 +0000 UTC m=+15064391.728315688.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.