

Acetamide, N-(2,5-dimethoxyphenyl)-2-methoxy-

Inchi: InChI=1S/C11H15NO4/c1-14-7-11(13)12-9-6-8(15-2)4-5-10(9)16-3/h4-6H,7H2,1-3H3,(H,
InchiKey: CJSLYAZJCWETED-UHFFFAOYSA-N
Formula: C11H15NO4
SMILES: COCC(O)=Nc1cc(OC)ccc1OC
Mol. weight [g/mol]: 225.24

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|--------|----------------|
| hf | -533.24 | kJ/mol | Joback Method |
| hvap | 70.98 | kJ/mol | Joback Method |
| log10ws | -1.60 | | Crippen Method |
| logp | 1.938 | | Crippen Method |
| mcvol | 171.250 | ml/mol | McGowan Method |
| pc | 2421.88 | kPa | Joback Method |
| rinpol | 1833.00 | | NIST Webbook |
| rinpol | 1833.00 | | NIST Webbook |
| tb | 723.72 | K | Joback Method |
| tc | 927.96 | K | Joback Method |

Sources

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U307261&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307I>
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method: https://en.wikipedia.org/wiki/Joback_method

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 |
| mcvol: | McGowan's characteristic volume |
| pc: | Critical Pressure |
| rinpol: | Non-polar retention indices |
| tb: | Normal Boiling Point Temperature |
| tc: | Critical Temperature |

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