

Methanimine, 1-(1-pyrrolidiny), N-(4-ethoxyphenyl)

Inchi: InChI=1S/C13H18N2O/c1-2-16-13-7-5-12(6-8-13)14-11-15-9-3-4-10-15/h5-8,11H,2-4,9-10H2
InchiKey: QOLGELLQSHMFEK-UHFFFAOYSA-N
Formula: C13H18N2O
SMILES: CCOc1ccc(N=CN2CCCC2)cc1
Mol. weight [g/mol]: 218.29

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|--------|----------------|
| log10ws | -2.79 | | Crippen Method |
| logp | 2.841 | | Crippen Method |
| mcvol | 180.940 | ml/mol | McGowan Method |
| rinpola | 2042.00 | | NIST Webbook |

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R118999&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
rinpola: Non-polar retention indices

Latest version available from:

<https://www.chemeo.com/cid/17-781-6/Methanimine-1-1-pyrrolidiny-N-4-ethoxyphenyl.pdf>

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