

Ethyl 3-pyridylacetate

| | |
|-----------------------------|---|
| Other names: | 3-Pyridineacetic acid, ethyl ester Acetic acid, 2-(3-pyridyl)-, ethyl ester Ethyl 3-pyridineacetate |
| Inchi: | InChI=1S/C9H11NO2/c1-2-12-9(11)6-8-4-3-5-10-7-8/h3-5,7H,2,6H2,1H3 |
| InchiKey: | RPWXYCRIAGBAGY-UHFFFAOYSA-N |
| Formula: | C9H11NO2 |
| SMILES: | CCOC(=O)Cc1ccnc1 |
| Mol. weight [g/mol]: | 165.19 |
| CAS: | 39931-77-6 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|--------|----------------|
| log10ws | -1.74 | | Crippen Method |
| logp | 1.187 | | Crippen Method |
| mcvol | 131.330 | ml/mol | McGowan Method |

Pressure Dependent Properties

| Property code | Value | Unit | Pressure [kPa] | Source |
|---------------|--------|------|----------------|--------------|
| tbrp | 353.20 | K | 0.05 | NIST Webbook |

Sources

| | |
|------------------------|---|
| McGowan Method: | http://link.springer.com/article/10.1007/BF02311772 |
| NIST Webbook: | http://webbook.nist.gov/cgi/cbook.cgi?ID=C39931776&Units=SI |
| Crippen Method: | http://pubs.acs.org/doi/abs/10.1021/ci9903071 |
| Crippen Method: | https://www.chemeo.com/doc/models/crippen_log10ws |

Legend

| | |
|-----------------|-------------------------------------|
| log10ws: | Log10 of Water solubility in mol/l |
| logp: | Octanol/Water partition coefficient |
| mcvol: | McGowan's characteristic volume |
| tbrp: | Boiling point at reduced pressure |

Latest version available from:

<https://www.cheméo.com/cid/16-898-8/Ethyl-3-pyridylacetate.pdf>

Generated by Cheméo on 2024-04-24 22:27:23.311231966 +0000 UTC m=+16286892.231809281.

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