

# 1-Piperidinepropanoic acid, ethyl ester

|                             |  |
|-----------------------------|--|
| <b>Other names:</b>         | Ethyl 1-piperidinepropionate<br>«beta»-(N-Piperidino)-propionic acid ethyl ester<br>1-Piperidinepropionic acid, ethyl ester<br>ethyl piperidine-1-propionate |
| <b>Inchi:</b>               | InChI=1S/C10H19NO2/c1-2-13-10(12)6-9-11-7-4-3-5-8-11/h2-9H2,1H3  |
| <b>InchiKey:</b>            | MPAWVDTVWPPKJQ-UHFFFAOYSA-N  |
| <b>Formula:</b>             | C10H19NO2  |
| <b>SMILES:</b>              | CCOC(=O)CCN1CCCCC1   |
| <b>Mol. weight [g/mol]:</b> | 185.26   |
| <b>CAS:</b>                 | 19653-33-9   |

## Physical Properties

| Property code | Value   | Unit   | Source         |
|---------------|---------|--------|----------------|
| log10ws       | -1.34   |        | Crippen Method |
| logp          | 1.425   |        | Crippen Method |
| mcvol         | 158.320 | ml/mol | McGowan Method |
| tb            | 491.20  | K      | NIST Webbook   |

## Sources

|                        |   |
|------------------------|---|
| <b>Crippen Method:</b> | <a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</a>                                     |
| <b>Crippen Method:</b> | <a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>                             |
| <b>McGowan Method:</b> | <a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>                         |
| <b>NIST Webbook:</b>   | <a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C19653339&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C19653339&amp;Units=SI</a> |

## Legend

|                 |                                     |
|-----------------|-------------------------------------|
| <b>log10ws:</b> | Log10 of Water solubility in mol/l  |
| <b>logp:</b>    | Octanol/Water partition coefficient |
| <b>mcvol:</b>   | McGowan's characteristic volume     |
| <b>tb:</b>      | Normal Boiling Point Temperature    |

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