

# (E)-1-(Piperidin-1-yl)tetradec-2-en-1-one

|                      |                                                                                    |
|----------------------|------------------------------------------------------------------------------------|
| Inchi:               | InChI=1S/C19H35NO/c1-2-3-4-5-6-7-8-9-10-11-13-16-19(21)20-17-14-12-15-18-20/h13,21 |
| InchiKey:            | JHTMREUWVSSNP-DTQAZKPQSA-N                                                         |
| Formula:             | C19H35NO                                                                           |
| SMILES:              | CCCCCCCCCCCC=CC(=O)N1CCCCC1                                                        |
| Mol. weight [g/mol]: | 293.49                                                                             |
| CAS:                 | 147030-04-4                                                                        |

## Physical Properties

| Property code | Value   | Unit   | Source         |
|---------------|---------|--------|----------------|
| log10ws       | -5.87   |        | Crippen Method |
| logp          | 5.476   |        | Crippen Method |
| mcvol         | 274.960 | ml/mol | McGowan Method |
| rinpol        | 2476.60 |        | NIST Webbook   |
| rinpol        | 2476.60 |        | NIST Webbook   |

## Sources

|                 |                                                                                                                                                 |
|-----------------|-------------------------------------------------------------------------------------------------------------------------------------------------|
| Crippen Method: | <a href="http://pubs.acs.org/doi/abs/10.1021/ci990307l">http://pubs.acs.org/doi/abs/10.1021/ci990307l</a>                                       |
| Crippen Method: | <a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>                               |
| McGowan Method: | <a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>                           |
| NIST Webbook:   | <a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C147030044&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C147030044&amp;Units=SI</a> |

## Legend

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

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